4H-CYCLOPENTA[DEF]PHENANTHRENE

Other names:	4,5-methylenephenanthrene 4,5-phenanthrylenemethane 4H-Cyclopenta[def]phenathrene 4H-Cyclopenta[drf]phenanthrene Cyclopenta[def]phenanthrene Methylenephenanthrene NSC 88888 Phenanthrene, 4,5-methylene- benzo[def]fluorene methane, 4,5-phenanthrylene-
Inchi:	InChI=1S/C15H10/c1-3-10-7-8-11-4-2-6-13-9-12(5-1)14(10)15(11)13/h1-8H,9H2
InchiKey:	RKZDZWJDQTZDLD-UHFFFAOYSA-N
Formula:	C15H10
SMILES:	c1cc2c3c(c1)ccc1cccc(c13)C2
Mol. weight [g/mol]:	190.25

Physical Properties

Property code	Value	Unit	Source
hf	259.27	kJ/mol	Cheméo Relay (1.0)
hfus	22.78	kJ/mol	Joback Method
hvap	83.40 ± 0.70	kJ/mol	NIST Webbook
ie	7.63	eV	Cheméo Relay (1.0)
log10ws	-6.05		Cheméo Relay (1.0)
logp	3.897		Crippen Method
mcvol	148.670	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	322.18		NIST Webbook
rinpol	325.73		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	318.60		NIST Webbook
rinpol	318.60		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	322.30		NIST Webbook
rinpol	322.64		NIST Webbook
rinpol	321.96		NIST Webbook
rinpol	322.52		NIST Webbook

rinpol	322.42		NIST Webbook
rinpol	322.02		NIST Webbook
rinpol	322.50		NIST Webbook
rinpol	321.96		NIST Webbook
rinpol	322.15		NIST Webbook
rinpol	321.77		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	325.73		NIST Webbook
rinpol	321.96		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	322.18		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	319.10		NIST Webbook
rinpol	319.50		NIST Webbook
rinpol	322.10		NIST Webbook
rinpol	322.30		NIST Webbook
rinpol	322.30		NIST Webbook
rinpol	319.53		NIST Webbook
rinpol	320.05		NIST Webbook
rinpol	321.05		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	322.82		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	322.08		NIST Webbook
rinpol	319.42		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1864.28		NIST Webbook
rinpol	1876.18		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1887.00		NIST Webbook
tb	646.40	K	Cheméo Relay (1.0)
tc	918.64	K	Cheméo Relay (1.0)
tf	406.62	K	Cheméo Relay (1.0)
vc	0.601	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.53	J/mol×K	875.79	Joback Method

cpg	373.26	J/mol×K	666.84	Joback Method
cpg	385.19	J/mol×K	708.63	Joback Method
cpg	360.17	J/mol×K	625.05	Joback Method
cpg	396.18	J/mol×K	750.42	Joback Method
cpg	406.43	J/mol×K	792.21	Joback Method
cpg	416.15	J/mol×K	834.00	Joback Method
dvisc	0.0017758	Pa×s	555.84	Joback Method
dvisc	0.0021397	Pa×s	417.41	Joback Method
dvisc	0.0020205	Pa×s	452.02	Joback Method
dvisc	0.0019236	Pa×s	486.62	Joback Method
dvisc	0.0018433	Pa×s	521.23	Joback Method
dvisc	0.0017182	Pa×s	590.44	Joback Method
dvisc	0.0016686	Pa×s	625.05	Joback Method
pvap	0.03	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.14	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.79	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.15	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.62	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.26	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.07	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.11	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.41	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.35	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.22	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.53	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.08	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.63e-05	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.96e-03	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.34e-03	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.51e-03	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	6.44e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.57e-04	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	9.50e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.24e-05	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Cheméo Relay (1.0, beta):

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C203645&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume