Phenanthrene-D10

Other names: Phenanthrene, perdeutero-
[2H10]Phenanthrene
Inchi: InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H/i1D,2D,3D,4D,5D,
InchiKey: YNPNZTXNASCQKK-LHNTUAQVSA-N
Formula: C14D10
SMILES: c1ccc2c(c1)ccc1ccccc12
Mol. weight [g/mol]: 188.29
CAS: 1517-22-2

Physical Properties

Property code	Value	Unit	Source
gf	383.08	kJ/mol	Joback Method
hf	274.91	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	78.60	kJ/mol	NIST Webbook
ie	8.05	eV	NIST Webbook
log10ws	-5.08		Crippen Method
logp	3.993		Crippen Method
mcvol	145.440	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1793.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	299.20		NIST Webbook
ripol	2713.00		NIST Webbook
tb	589.34	K	Joback Method
tc	843.18	K	Joback Method
tf	351.88	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.65	J/mol×K	843.18	Joback Method

cpg	334.16	J/mol×K	589.34	Joback Method
cpg	349.09	J/mol×K	631.65	Joback Method
cpg	362.69	J/mol×K	673.95	Joback Method
cpg	375.10	J/mol×K	716.26	Joback Method
cpg	386.47	J/mol×K	758.56	Joback Method
cpg	396.94	J/mol×K	800.87	Joback Method
dvisc	0.0004678	Pa×s	589.34	Joback Method
dvisc	0.0014969	Pa×s	351.88	Joback Method
dvisc	0.0011180	Pa×s	391.46	Joback Method
dvisc	0.0008810	Pa×s	431.03	Joback Method
dvisc	0.0007226	Pa×s	470.61	Joback Method
dvisc	0.0006112	Pa×s	510.19	Joback Method
dvisc	0.0005296	Pa×s	549.76	Joback Method
hsubt	92.20 ± 1.10	kJ/mol	303.00	NIST Webbook
hvapt	78.62	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects: https://www.doi.org/10.1021/je800091s

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004229&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume