

Phenanthrene, 3-methyl-

Other names:	3-Methylphenanthrene 3-Methylphenanthrene
Inchi:	InChI=1S/C15H12/c1-11-6-7-13-9-8-12-4-2-3-5-14(12)15(13)10-11/h2-10H,1H3
InchiKey:	GKYWZUBZZBHZKU-UHFFFAOYSA-N
Formula:	C15H12
SMILES:	<chem>Cc1ccc2ccc3ccccc3c2c1</chem>
Mol. weight [g/mol]:	192.26
CAS:	832-71-3

Physical Properties

Property code	Value	Unit	Source
gf	381.87	kJ/mol	Joback Method
hf	242.80	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
ie	7.68 ± 0.01	eV	NIST Webbook
log10ws	-5.56		Crippen Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1879.60		NIST Webbook
rinpol	1909.30		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	318.85		NIST Webbook
rinpol	319.46		NIST Webbook
rinpol	318.60		NIST Webbook
rinpol	318.93		NIST Webbook
rinpol	317.58		NIST Webbook
rinpol	319.08		NIST Webbook
rinpol	318.88		NIST Webbook
rinpol	319.04		NIST Webbook

rinpol	318.61		NIST Webbook
rinpol	319.40		NIST Webbook
rinpol	319.40		NIST Webbook
rinpol	319.34		NIST Webbook
rinpol	319.54		NIST Webbook
rinpol	319.03		NIST Webbook
rinpol	318.90		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	319.06		NIST Webbook
rinpol	319.19		NIST Webbook
rinpol	319.46		NIST Webbook
rinpol	318.83		NIST Webbook
rinpol	318.83		NIST Webbook
rinpol	318.93		NIST Webbook
rinpol	319.03		NIST Webbook
rinpol	315.60		NIST Webbook
rinpol	318.17		NIST Webbook
rinpol	315.60		NIST Webbook
rinpol	318.60		NIST Webbook
rinpol	319.50		NIST Webbook
rinpol	318.60		NIST Webbook
rinpol	319.46		NIST Webbook
rinpol	318.22		NIST Webbook
rinpol	317.70		NIST Webbook
rinpol	319.20		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	315.61		NIST Webbook
rinpol	319.46		NIST Webbook
rinpol	319.55		NIST Webbook
rinpol	315.00		NIST Webbook
rinpol	316.35		NIST Webbook
rinpol	319.46		NIST Webbook
rinpol	318.83		NIST Webbook
rinpol	318.17		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	315.61		NIST Webbook
rinpol	318.93		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	319.46		NIST Webbook
tb	617.20	K	Joback Method
tc	866.35	K	Joback Method
tf	375.67	K	Joback Method

vc

0.612

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	617.20	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
cpg	456.90	J/mol×K	866.35	Joback Method
dvisc	0.0004506	Paxs	617.20	Joback Method
dvisc	0.0005079	Paxs	576.95	Joback Method
dvisc	0.0005828	Paxs	536.69	Joback Method
dvisc	0.0006839	Paxs	496.44	Joback Method
dvisc	0.0008255	Paxs	456.18	Joback Method
dvisc	0.0010334	Paxs	415.93	Joback Method
dvisc	0.0013574	Paxs	375.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36552e+01
Coeff. B	-4.62698e+03
Coeff. C	-1.14386e+02
Temperature range (K), min.	460.52
Temperature range (K), max.	668.93

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C832713&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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