

Phenanthrene, 1,2,3,4-tetrahydro-

Other names:	1,2,3,4-Tetrahydrophenanthrene
Inchi:	InChI=1S/C14H14/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1,3,5,7,9-10H,2,4,6,8H2
InchiKey:	UXNCDAQNSQBHEN-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	c1ccc2c3c(ccc2c1)CCCC3
Mol. weight [g/mol]:	182.26
CAS:	1013-08-7

Physical Properties

Property code	Value	Unit	Source
gf	323.16	kJ/mol	Joback Method
hf	92.30 ± 1.30	kJ/mol	NIST Webbook
hfus	17.26	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.719		Crippen Method
mcvol	154.040	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	297.21		NIST Webbook
rinpol	1767.70		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	297.21		NIST Webbook
rinpol	296.00		NIST Webbook
rinpol	1755.20		NIST Webbook
rinpol	1755.20		NIST Webbook
rinpol	1737.60		NIST Webbook
rinpol	1767.70		NIST Webbook
rinpol	1767.70		NIST Webbook
rinpol	1737.60		NIST Webbook
rinpol	1737.60		NIST Webbook
rinpol	1772.00		NIST Webbook
sl	286.60	J/mol×K	NIST Webbook
tb	591.02	K	Joback Method
tc	839.70	K	Joback Method
tf	350.36	K	Joback Method
tt	302.55 ± 0.01	K	NIST Webbook
tt	302.56 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.46	J/mol×K	839.70	Joback Method
cpg	408.48	J/mol×K	673.91	Joback Method
cpg	423.32	J/mol×K	715.36	Joback Method
cpg	437.01	J/mol×K	756.81	Joback Method
cpg	449.68	J/mol×K	798.26	Joback Method
cpg	392.34	J/mol×K	632.47	Joback Method
cpg	374.79	J/mol×K	591.02	Joback Method
cpl	278.26	J/mol×K	298.15	NIST Webbook
dvisc	0.0004484	Pa×s	591.02	Joback Method
dvisc	0.0006180	Pa×s	510.80	Joback Method
dvisc	0.0007558	Pa×s	470.69	Joback Method
dvisc	0.0009598	Pa×s	430.58	Joback Method
dvisc	0.0012802	Pa×s	390.47	Joback Method
dvisc	0.0005203	Pa×s	550.91	Joback Method
dvisc	0.0018238	Pa×s	350.36	Joback Method
hfust	1.77	kJ/mol	298.00	NIST Webbook
hfust	5.83	kJ/mol	285.00	NIST Webbook
hfust	11.17	kJ/mol	302.60	NIST Webbook
sfust	5.92	J/mol×K	298.00	NIST Webbook
sfust	20.44	J/mol×K	285.00	NIST Webbook
sfust	36.91	J/mol×K	302.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.20	K	1.50	NIST Webbook

Sources

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=C1013087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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