

Pyracene

Inchi:	InChI=1S/C14H12/c1-2-10-7-8-12-4-3-11-6-5-9(1)13(10)14(11)12/h5-8H,1-4H2
InchiKey:	UUBIWGRMBVAUIK-UHFFFAOYSA-N
Formula:	C14H12
SMILES:	<chem>c1cc2c3c(ccc4c3c1CC4)CC2</chem>
Mol. weight [g/mol]:	180.25
CAS:	567-79-3

Physical Properties

Property code	Value	Unit	Source
gf	408.66	kJ/mol	Joback Method
hf	174.30 ± 5.30	kJ/mol	NIST Webbook
hfs	84.70 ± 4.10	kJ/mol	NIST Webbook
hfus	19.85	kJ/mol	Joback Method
hsub	89.60 ± 3.30	kJ/mol	NIST Webbook
hvap	53.42	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.037		Crippen Method
mvol	143.180	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	599.58	K	Joback Method
tc	842.23	K	Joback Method
tf	408.14	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.77	J/mol×K	599.58	Joback Method
cpg	367.87	J/mol×K	640.02	Joback Method
cpg	380.78	J/mol×K	680.46	Joback Method
cpg	392.68	J/mol×K	720.91	Joback Method
cpg	403.77	J/mol×K	761.35	Joback Method
cpg	414.23	J/mol×K	801.79	Joback Method
cpg	424.25	J/mol×K	842.23	Joback Method

dvisc	0.0023477	Paxs	408.14	Joback Method
dvisc	0.0022672	Paxs	440.05	Joback Method
dvisc	0.0021998	Paxs	471.95	Joback Method
dvisc	0.0021426	Paxs	503.86	Joback Method
dvisc	0.0020934	Paxs	535.77	Joback Method
dvisc	0.0020507	Paxs	567.67	Joback Method
dvisc	0.0020133	Paxs	599.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C567793&Units=SI
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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