Nigritene

Inchi: InChI=1S/C14H22/c1-10-13(2,3)11-6-8-14(10)7-4-5-12(14)9-11/h5,10-11H,4,6-9H2,1-3H
InchiKey: AHSSPFZOPLOXCJ-UHFFFAOYSA-N
Formula: C14H22
SMILES: CC1C23CCC=C2CC(CC3)C1(C)C
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	226.69	kJ/mol	Joback Method
hf	-69.76	kJ/mol	Joback Method
hfus	11.53	kJ/mol	Joback Method
hvap	45.18	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.169		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1387.00		NIST Webbook
tb	548.43	K	Joback Method
tc	778.30	K	Joback Method
tf	351.16	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.53	J/mol×K	548.43	Joback Method
cpg	473.78	J/mol×K	586.74	Joback Method
cpg	494.32	J/mol×K	625.05	Joback Method
cpg	513.49	J/mol×K	663.37	Joback Method
cpg	531.58	J/mol×K	701.68	Joback Method
cpg	548.92	J/mol×K	739.99	Joback Method
cpg	565.83	J/mol×K	778.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R516244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume