Dehydronigritene

Inchi: InChI=1S/C14H20/c1-10-13(2,3)11-6-8-14(10)7-4-5-12(14)9-11/h5,11H,1,4,6-9H2,2-3H3
InchiKey: UEWFRELXRTUKOE-UHFFFAOYSA-N
Formula: C14H20
SMILES: C=C1C23CCC=C2CC(CC3)C1(C)C
Mol. weight [g/mol]: 188.31

Physical Properties

Property code	Value	Unit	Source
gf	287.48	kJ/mol	Joback Method
hf	34.82	kJ/mol	Joback Method
hfus	9.30	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.089		Crippen Method
mcvol	166.940	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
tb	552.26	K	Joback Method
tc	784.26	K	Joback Method
tf	369.08	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.06	J/mol×K	552.26	Joback Method
cpg	451.40	J/mol×K	590.93	Joback Method
cpg	470.15	J/mol×K	629.59	Joback Method
cpg	487.63	J/mol×K	668.26	Joback Method
cpg	504.17	J/mol×K	706.93	Joback Method
cpg	520.10	J/mol×K	745.59	Joback Method
cpg	535.73	J/mol×K	784.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R516239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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