

dehydroionene

Inchi: InChI=1S/C13H18/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-9H,1,10H2,2-4H3/b9-6+
InchiKey: ACFCPKXNISJZKZ-RMKNXTFCSA-N
Formula: C13H18
SMILES: C=CC=CC1=C(C)C=CCC1(C)C
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
gf	286.26	kJ/mol	Joback Method
hf	93.18	kJ/mol	Joback Method
hfus	15.55	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.031		Crippen Method
mcvol	165.970	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1348.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1682.00		NIST Webbook
tb	525.75	K	Joback Method
tc	743.38	K	Joback Method
tf	287.27	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.05	J/molxK	525.75	Joback Method
cpg	392.81	J/molxK	562.02	Joback Method
cpg	409.41	J/molxK	598.29	Joback Method
cpg	424.97	J/molxK	634.56	Joback Method

cpg	439.63	J/mol×K	670.83	Joback Method
cpg	453.54	J/mol×K	707.11	Joback Method
cpg	466.82	J/mol×K	743.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R239833&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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