

Spiro[8,8-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalene]

Inchi: InChI=1S/C16H24O/c1-15(2)8-3-5-12-7-10-16(11-13(12)15)9-4-6-14(16)17/h3-11H2,1-2H1
InchiKey: GQMLSYHTNXNKQK-UHFFFAOYSA-N
Formula: C16H24O
SMILES: CC1(C)CCCC2=C1CC1(CCCC1=O)CC2
Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
gf	90.43	kJ/mol	Joback Method
hf	-238.01	kJ/mol	Joback Method
hfus	7.39	kJ/mol	Joback Method
hvap	55.68	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.416		Crippen Method
mcvol	200.990	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1822.40		NIST Webbook
rinpol	1832.30		NIST Webbook
rinpol	1822.40		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2335.70		NIST Webbook
ripol	2320.00		NIST Webbook
tb	689.14	K	Joback Method
tc	947.32	K	Joback Method
tf	452.36	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.33	J/molxK	689.14	Joback Method
cpg	622.91	J/molxK	732.17	Joback Method
cpg	645.52	J/molxK	775.20	Joback Method
cpg	667.53	J/molxK	818.23	Joback Method

cpg	689.32	J/mol×K	861.26	Joback Method
cpg	711.29	J/mol×K	904.29	Joback Method
cpg	733.79	J/mol×K	947.32	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=R179558&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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