C16-Homodrimane

Inchi: InChI=1S/C16H30/c1-11-9-15(4,5)14-8-7-12(2)13(3)16(14,6)10-11/h11-14H,7-10H2,1-6H
InchiKey: OTKVIAFXSNFZKS-HDXBLWQJSA-N
Formula: C16H30
SMILES: CC1CC(C)(C)C2CCC(C)C(C)C2(C)C1
Mol. weight [g/mol]: 222.41

Physical Properties

Property code	Value	Unit	Source
gf	115.12	kJ/mol	Joback Method
hf	-303.49	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	48.19	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	5.131		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	1567.00		NIST Webbook
tb	577.84	K	Joback Method
tc	795.50	K	Joback Method
tf	322.72	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.64	J/mol×K	577.84	Joback Method
cpg	620.38	J/mol×K	614.12	Joback Method
cpg	645.59	J/mol×K	650.39	Joback Method
cpg	669.49	J/mol×K	686.67	Joback Method
cpg	692.29	J/mol×K	722.95	Joback Method
cpg	714.21	J/mol×K	759.22	Joback Method
cpg	735.44	J/mol×K	795.50	Joback Method

Sources

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=R548657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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