8-«beta»(H)-Homodrimane

Inchi: InChI=1S/C16H30/c1-6-13-12(2)8-9-14-15(3,4)10-7-11-16(13,14)5/h12-14H,6-11H2,1-5H
InchiKey: PXIHFQXAITTXJK-RZLSGREXSA-N
Formula: C16H30
SMILES: CCC1C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 222.41

Physical Properties

Property code	Value	Unit	Source
gf	122.83	kJ/mol	Joback Method
hf	-283.15	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.275		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1539.00		NIST Webbook
tb	582.51	K	Joback Method
tc	800.21	K	Joback Method
tf	326.96	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.44	J/mol×K	582.51	Joback Method
cpg	619.62	J/mol×K	618.79	Joback Method
cpg	644.31	J/mol×K	655.08	Joback Method
cpg	667.70	J/mol×K	691.36	Joback Method
cpg	690.04	J/mol×K	727.65	Joback Method
cpg	711.53	J/mol×K	763.93	Joback Method
cpg	732.39	J/mol×K	800.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591394&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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