heterotactic-2,4,6,8,10-Pentamethyl-1,10-undecad

Inchi: InChI=1S/C16H30/c1-12(2)8-14(5)10-16(7)11-15(6)9-13(3)4/h14-16H,1,3,8-11H2,2,4-7H
InchiKey: CFISLIQCGZWQLG-UHFFFAOYSA-N
Formula: C16H30
SMILES: C=C(C)CC(C)CC(C)CC(C)CC(=C)C
Mol. weight [g/mol]: 222.41

Physical Properties

Property code	Value	Unit	Source
gf	235.10	kJ/mol	Joback Method
hf	-158.13	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.607		Crippen Method
mcvol	227.700	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	1392.00		NIST Webbook
tb	557.28	K	Joback Method
tc	734.59	K	Joback Method
tf	193.64	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.48	J/mol×K	557.28	Joback Method
cpg	590.47	J/mol×K	586.83	Joback Method
cpg	609.54	J/mol×K	616.38	Joback Method
cpg	627.72	J/mol×K	645.93	Joback Method
cpg	645.05	J/mol×K	675.49	Joback Method
cpg	661.56	J/mol×K	705.04	Joback Method
cpg	677.29	J/mol×K	734.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628476&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume