2-cis,6-cis-Farnesol

Inchi: InChI=1S/C16H28/c1-6-9-15(4)12-8-13-16(5)11-7-10-14(2)3/h9-10,13H,6-8,11-12H2,1-5
InchiKey: XVIPCWLIFRBCRP-KKYYKMBRSA-N
Formula: C16H28
SMILES: CCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 220.39

Physical Properties

Property code	Value	Unit	Source
gf	298.85	kJ/mol	Joback Method
hf	-51.28	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.816		Crippen Method
mcvol	223.400	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	577.60	K	Joback Method
tc	762.59	K	Joback Method
tf	212.96	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.77	J/mol×K	577.60	Joback Method
cpg	574.82	J/mol×K	608.43	Joback Method
cpg	592.91	J/mol×K	639.26	Joback Method
cpg	610.09	J/mol×K	670.10	Joback Method
cpg	626.42	J/mol×K	700.93	Joback Method
cpg	641.95	J/mol×K	731.76	Joback Method
cpg	656.75	J/mol×K	762.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285202&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

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