(E)-2,3-Dihydrofarnesal

Inchi: InChI=1S/C15H26O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,12,15H,5-6,8,10-11H
InchiKey: ITBYWGRSPHMAEE-NTEUORMPSA-N
Formula: C15H26O
SMILES: CC(C)=CCCC(C)=CCCC(C)CC=O
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	116.80	kJ/mol	Joback Method
hf	-228.93	kJ/mol	Joback Method
hfus	31.16	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.684		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	598.90	K	Joback Method
tc	783.10	K	Joback Method
tf	247.73	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.05	J/mol×K	598.90	Joback Method
cpg	568.45	J/mol×K	629.60	Joback Method
cpg	584.98	J/mol×K	660.30	Joback Method
cpg	600.68	J/mol×K	691.00	Joback Method
cpg	615.60	J/mol×K	721.70	Joback Method
cpg	629.78	J/mol×K	752.40	Joback Method
cpg	643.27	J/mol×K	783.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324822&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