Farnesyl butanoate

Inchi: InChI=1S/C19H32O2/c1-6-9-19(20)21-15-14-18(5)13-8-12-17(4)11-7-10-16(2)3/h10,12,1
InchiKey: GPNSLSVRBMEOCK-NXGXIAAHSA-N
Formula: C19H32O2
SMILES: CCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 292.46
CAS: 51532-27-5

Physical Properties

Property code	Value	Unit	Source
gf	90.19	kJ/mol	Joback Method
hf	-358.00	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.749		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	2019.90		NIST Webbook
rinpol	2019.90		NIST Webbook
tb	722.53	K	Joback Method
tc	910.02	K	Joback Method
tf	318.93	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.43	J/mol×K	722.53	Joback Method
cpg	797.72	J/mol×K	753.78	Joback Method
cpg	815.09	J/mol×K	785.03	Joback Method
cpg	831.62	J/mol×K	816.27	Joback Method
cpg	847.35	J/mol×K	847.52	Joback Method
cpg	862.34	J/mol×K	878.77	Joback Method
cpg	876.65	J/mol×K	910.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51532275&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