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-UHFFFAOYSA-N
Formula: C19H32O2
SMILES: CCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 292.46

Physical Properties

Property code	Value	Unit	Source
af	0.6506		Cheméo Relay (1.0)
hf	-551.85	kJ/mol	Cheméo Relay (1.0)
hfus	44.43	kJ/mol	Joback Method
hvap	88.65	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.41		Cheméo Relay (1.0)
logp	5.749		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	580.96	K	Cheméo Relay (1.0)
tc	752.82	K	Cheméo Relay (1.0)
tf	224.58	K	Cheméo Relay (1.0)
vc	0.970	m3/kmol	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R239888&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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