(E, E)-farnesyl 3-methylbutanoate

Inchi: InChI=1S/C20H34O2/c1-16(2)9-7-10-18(5)11-8-12-19(6)13-14-22-20(21)15-17(3)4/h9,11
InchiKey: BZQKWZWRJMKCNP-NWLVNBMCSA-N
Formula: C20H34O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCOC(=O)CC(C)C
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	96.17	kJ/mol	Joback Method
hf	-383.92	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.995		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	744.97	K	Joback Method
tc	934.31	K	Joback Method
tf	315.20	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.99	J/mol×K	744.97	Joback Method
cpg	856.83	J/mol×K	776.53	Joback Method
cpg	874.73	J/mol×K	808.08	Joback Method
cpg	891.74	J/mol×K	839.64	Joback Method
cpg	907.93	J/mol×K	871.20	Joback Method
cpg	923.34	J/mol×K	902.76	Joback Method
cpg	938.05	J/mol×K	934.31	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=R420341&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