dihydrofarnesyl pentanoate

Inchi: InChI=1S/C20H36O2/c1-6-7-14-20(21)22-16-15-19(5)13-9-12-18(4)11-8-10-17(2)3/h10,1
InchiKey: TTXHHXWCLVQXSE-XDJHFCHBSA-N
Formula: C20H36O2
SMILES: CCCCC(=O)OCC=C(C)CCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 308.50

Physical Properties

Property code	Value	Unit	Source
gf	24.50	kJ/mol	Joback Method
hf	-491.35	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.219		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	740.93	K	Joback Method
tc	923.80	K	Joback Method
tf	334.24	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.88	J/mol×K	740.93	Joback Method
cpg	881.00	J/mol×K	771.41	Joback Method
cpg	899.18	J/mol×K	801.89	Joback Method
cpg	916.47	J/mol×K	832.37	Joback Method
cpg	932.90	J/mol×K	862.84	Joback Method
cpg	948.53	J/mol×K	893.32	Joback Method
cpg	963.39	J/mol×K	923.80	Joback Method

Sources

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=R300831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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