(Z,E)-Farnesyl caproate

Inchi: InChI=1S/C21H36O2/c1-6-7-8-15-21(22)23-17-16-20(5)14-10-13-19(4)12-9-11-18(2)3/h1
InchiKey: RLRVQTPROCYANT-QBAIPTAWSA-N
Formula: C21H36O2
SMILES: CCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-399.28	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.529		Crippen Method
mcvol	301.290	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
ripol	2436.00		NIST Webbook
tb	768.29	K	Joback Method
tc	955.62	K	Joback Method
tf	341.47	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.62	J/mol×K	768.29	Joback Method
cpg	915.56	J/mol×K	799.51	Joback Method
cpg	933.58	J/mol×K	830.73	Joback Method
cpg	950.73	J/mol×K	861.96	Joback Method
cpg	967.07	J/mol×K	893.18	Joback Method
cpg	982.67	J/mol×K	924.40	Joback Method
cpg	997.58	J/mol×K	955.62	Joback Method

Sources

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=R517470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume