(Z,E)-Farnesyl caprylate

Inchi: InChI=1S/C23H40O2/c1-6-7-8-9-10-17-23(24)25-19-18-22(5)16-12-15-21(4)14-11-13-20
InchiKey: HHSVAJNBWYMLPB-AAYKTNCRSA-N
Formula: C23H40O2
SMILES: CCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 348.56

Physical Properties

Property code	Value	Unit	Source
gf	123.87	kJ/mol	Joback Method
hf	-440.56	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	76.06	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.309		Crippen Method
mcvol	329.470	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
ripol	2627.00		NIST Webbook
ripol	2627.00		NIST Webbook
tb	814.05	K	Joback Method
tc	1003.63	K	Joback Method
tf	364.01	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.65	J/mol×K	814.05	Joback Method
cpg	1037.32	J/mol×K	845.65	Joback Method
cpg	1056.02	J/mol×K	877.24	Joback Method
cpg	1073.84	J/mol×K	908.84	Joback Method
cpg	1090.84	J/mol×K	940.44	Joback Method
cpg	1107.08	J/mol×K	972.03	Joback Method
cpg	1122.63	J/mol×K	1003.63	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=R517485&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