(Z,Z)-Farnesyl caprate

Inchi: InChI=1S/C25H44O2/c1-6-7-8-9-10-11-12-19-25(26)27-21-20-24(5)18-14-17-23(4)16-13
InchiKey: ZSPZCKNQANJUIH-XVIBSYCRSA-N
Formula: C25H44O2
SMILES: CCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 376.62

Physical Properties

Property code	Value	Unit	Source
gf	140.71	kJ/mol	Joback Method
hf	-481.84	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.090		Crippen Method
mcvol	357.650	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
ripol	2801.00		NIST Webbook
ripol	2801.00		NIST Webbook
tb	859.81	K	Joback Method
tc	1054.48	K	Joback Method
tf	386.55	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.06	J/mol×K	859.81	Joback Method
cpg	1162.60	J/mol×K	892.26	Joback Method
cpg	1182.14	J/mol×K	924.70	Joback Method
cpg	1200.76	J/mol×K	957.15	Joback Method
cpg	1218.53	J/mol×K	989.59	Joback Method
cpg	1235.53	J/mol×K	1022.04	Joback Method
cpg	1251.84	J/mol×K	1054.48	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=R517509&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