2,3-Dihydrofarnesyl decanoate

Inchi: InChI=1S/C25H46O2/c1-6-7-8-9-10-11-12-19-25(26)27-21-20-24(5)18-14-17-23(4)16-13
InchiKey: GQOWPKZBFFQEEF-HAVVHWLPSA-N
Formula: C25H46O2
SMILES: CCCCCCCCCC(=O)OCCC(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 378.63
CAS: 220284-39-9

Physical Properties

Property code	Value	Unit	Source
gf	66.60	kJ/mol	Joback Method
hf	-594.55	kJ/mol	Joback Method
hfus	57.55	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	8.169		Crippen Method
mcvol	361.950	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2562.20		NIST Webbook
tb	855.33	K	Joback Method
tc	1048.10	K	Joback Method
tf	390.59	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1168.90	J/mol×K	855.33	Joback Method
cpg	1189.94	J/mol×K	887.46	Joback Method
cpg	1209.89	J/mol×K	919.59	Joback Method
cpg	1228.81	J/mol×K	951.71	Joback Method
cpg	1246.77	J/mol×K	983.84	Joback Method
cpg	1263.82	J/mol×K	1015.97	Joback Method
cpg	1280.04	J/mol×K	1048.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220284399&Units=SI
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

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