(2E,6E)-Farnesyl pentanoate

Inchi: InChI=1S/C20H34O2/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: WLNFGKOLWOXXAF-XYAZGONESA-N
Formula: C20H34O2
SMILES: CCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 306.48
CAS: 126182-13-6

Physical Properties

Property code	Value	Unit	Source
gf	98.61	kJ/mol	Joback Method
hf	-378.64	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	69.38	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.139		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	2063.40		NIST Webbook
rinpol	2063.40		NIST Webbook
tb	745.41	K	Joback Method
tc	932.54	K	Joback Method
tf	330.20	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.52	J/mol×K	745.41	Joback Method
cpg	856.12	J/mol×K	776.60	Joback Method
cpg	873.82	J/mol×K	807.79	Joback Method
cpg	890.66	J/mol×K	838.98	Joback Method
cpg	906.69	J/mol×K	870.17	Joback Method
cpg	921.99	J/mol×K	901.36	Joback Method
cpg	936.60	J/mol×K	932.54	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=C126182136&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

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