

geranyl levulinate

Inchi:	InChI=1S/C15H24O3/c1-12(2)6-5-7-13(3)10-11-18-15(17)9-8-14(4)16/h6,10H,5,7-9,11H2
InchiKey:	LYZVOWORCQDZCM-JLHYYAGUSA-N
Formula:	C15H24O3
SMILES:	CC(=O)CCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	252.35

Physical Properties

Property code	Value	Unit	Source
gf	-144.08	kJ/mol	Joback Method
hf	-495.45	kJ/mol	Joback Method
hfus	36.78	kJ/mol	Joback Method
hvap	64.96	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.591		Crippen Method
mcvol	222.620	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
ripol	2504.00		NIST Webbook
tb	680.84	K	Joback Method
tc	871.91	K	Joback Method
tf	342.82	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.11	J/molxK	680.84	Joback Method
cpg	618.82	J/molxK	712.69	Joback Method
cpg	633.70	J/molxK	744.53	Joback Method
cpg	647.81	J/molxK	776.38	Joback Method
cpg	661.17	J/molxK	808.22	Joback Method
cpg	673.83	J/molxK	840.07	Joback Method
cpg	685.82	J/molxK	871.91	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=R321452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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