Geranyl octanoate

Inchi: InChI=1S/C18H32O2/c1-5-6-7-8-9-13-18(19)20-15-14-17(4)12-10-11-16(2)3/h11,14H,5-1
InchiKey: YYBMOGCOPQVSLQ-SAPNQHFASA-N
Formula: C18H32O2
SMILES: CCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 280.45
CAS: 51532-26-4

Physical Properties

Property code	Value	Unit	Source
gf	10.10	kJ/mol	Joback Method
hf	-444.79	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	64.89	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.583		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1953.10		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	695.61	K	Joback Method
tc	876.41	K	Joback Method
tf	326.70	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.18	J/mol×K	695.61	Joback Method
cpg	763.38	J/mol×K	725.74	Joback Method
cpg	780.71	J/mol×K	755.88	Joback Method
cpg	797.21	J/mol×K	786.01	Joback Method
cpg	812.91	J/mol×K	816.14	Joback Method
cpg	827.86	J/mol×K	846.28	Joback Method
cpg	842.09	J/mol×K	876.41	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51532264&Units=SI

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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