Citronellyl heptanoate

Inchi: InChI=1S/C17H32O2/c1-5-6-7-8-12-17(18)19-14-13-16(4)11-9-10-15(2)3/h10,16H,5-9,11
InchiKey: JZTNHMKNNVAGPD-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 268.43
CAS: 72934-17-9

Physical Properties

Property code	Value	Unit	Source
gf	-72.43	kJ/mol	Joback Method
hf	-536.86	kJ/mol	Joback Method
hfus	37.94	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.273		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1820.30		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1820.30		NIST Webbook
tb	668.25	K	Joback Method
tc	844.66	K	Joback Method
tf	319.47	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.05	J/mol×K	668.25	Joback Method
cpg	729.41	J/mol×K	697.65	Joback Method
cpg	746.91	J/mol×K	727.05	Joback Method

cpg	763.59	J/mol×K	756.46	Joback Method
cpg	779.47	J/mol×K	785.86	Joback Method
cpg	794.58	J/mol×K	815.26	Joback Method
cpg	808.95	J/mol×K	844.66	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=C72934179&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