Citronellyl isoheptanoate

Inchi: InChI=1S/C17H32O2/c1-14(2)8-6-10-16(5)12-13-19-17(18)11-7-9-15(3)4/h8,15-16H,6-7,
InchiKey: QUYHAHHJNGZYSG-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CC(C)=CCCC(C)CCOC(=O)CCCC(C)C
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-74.87	kJ/mol	Joback Method
hf	-542.14	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.128		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	667.81	K	Joback Method
tc	846.67	K	Joback Method
tf	304.47	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.47	J/mol×K	667.81	Joback Method
cpg	730.11	J/mol×K	697.62	Joback Method
cpg	747.87	J/mol×K	727.43	Joback Method
cpg	764.77	J/mol×K	757.24	Joback Method
cpg	780.85	J/mol×K	787.05	Joback Method
cpg	796.12	J/mol×K	816.86	Joback Method
cpg	810.63	J/mol×K	846.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200627&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