Lauric acid, cyclohexylmethyl ester

Inchi: InChI=1S/C19H36O2/c1-2-3-4-5-6-7-8-9-13-16-19(20)21-17-18-14-11-10-12-15-18/h18H
InchiKey: VHTNBSNRTWIBSL-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: CCCCCCCCCCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-100.37	kJ/mol	Joback Method
hf	-625.97	kJ/mol	Joback Method
hfus	39.59	kJ/mol	Joback Method
hvap	67.47	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.031		Crippen Method
mcvol	275.150	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	2163.00		NIST Webbook
tb	729.96	K	Joback Method
tc	916.79	K	Joback Method
tf	383.43	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.17	J/mol×K	729.96	Joback Method
cpg	867.17	J/mol×K	761.10	Joback Method
cpg	887.03	J/mol×K	792.24	Joback Method
cpg	905.76	J/mol×K	823.37	Joback Method
cpg	923.39	J/mol×K	854.51	Joback Method
cpg	939.96	J/mol×K	885.65	Joback Method
cpg	955.50	J/mol×K	916.79	Joback Method
dvisc	0.0021704	Pa×s	383.43	Joback Method
dvisc	0.0008958	Pa×s	441.19	Joback Method

dvisc	0.0004538	Pa×s	498.94	Joback Method
dvisc	0.0002647	Pa×s	556.69	Joback Method
dvisc	0.0001709	Pa×s	614.45	Joback Method
dvisc	0.0001189	Pa×s	672.20	Joback Method
dvisc	0.0000877	Pa×s	729.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357925&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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