

Cyclohexyl tridecanoate

Inchi:	InChI=1S/C19H36O2/c1-2-3-4-5-6-7-8-9-10-14-17-19(20)21-18-15-12-11-13-16-18/h18H
InchiKey:	WXCHSMQQILPIJC-UHFFFAOYSA-N
Formula:	C19H36O2
SMILES:	CCCCCCCCCCCC(=O)OC1CCCCC1
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	-6.64		Crippen Method
logp	6.173		Crippen Method
mvol	275.150	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	2113.00		NIST Webbook
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tb	729.96	K	Joback Method
tc	916.79	K	Joback Method
tf	383.43	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.17	J/molxK	729.96	Joback Method
cpg	939.96	J/molxK	885.65	Joback Method
cpg	923.39	J/molxK	854.51	Joback Method
cpg	905.76	J/molxK	823.37	Joback Method
cpg	887.03	J/molxK	792.24	Joback Method
cpg	867.17	J/molxK	761.10	Joback Method
cpg	955.50	J/molxK	916.79	Joback Method
dvisc	0.0000877	Paxs	729.96	Joback Method

dvisc	0.0001189	Paxs	672.20	Joback Method
dvisc	0.0001709	Paxs	614.45	Joback Method
dvisc	0.0002647	Paxs	556.69	Joback Method
dvisc	0.0004538	Paxs	498.94	Joback Method
dvisc	0.0008958	Paxs	441.19	Joback Method
dvisc	0.0021704	Paxs	383.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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