

Octanoic acid, cyclohexyl ester

Other names:	Cyclohexyl caprylate
Inchi:	InChI=1S/C14H26O2/c1-2-3-4-5-9-12-14(15)16-13-10-7-6-8-11-13/h13H,2-12H2,1H3
InchiKey:	TXWXLLMVRVKQSO-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	226.35
CAS:	1551-42-4

Physical Properties

Property code	Value	Unit	Source
gf	-142.47	kJ/mol	Joback Method
hf	-522.77	kJ/mol	Joback Method
hfus	26.64	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.223		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	615.56	K	Joback Method
tc	809.77	K	Joback Method
tf	327.08	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.97	J/molxK	615.56	Joback Method
cpg	579.88	J/molxK	647.93	Joback Method
cpg	598.76	J/molxK	680.30	Joback Method
cpg	616.63	J/molxK	712.67	Joback Method
cpg	633.51	J/molxK	745.04	Joback Method
cpg	649.42	J/molxK	777.41	Joback Method

cpg	664.38	J/molxK	809.77	Joback Method
dvisc	0.0034050	Paxs	327.08	Joback Method
dvisc	0.0014830	Paxs	375.16	Joback Method
dvisc	0.0007802	Paxs	423.24	Joback Method
dvisc	0.0004679	Paxs	471.32	Joback Method
dvisc	0.0003085	Paxs	519.40	Joback Method
dvisc	0.0002182	Paxs	567.48	Joback Method
dvisc	0.0001630	Paxs	615.56	Joback Method

Sources

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=C1551424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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