

Cyclohexanecarboxylic acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C15H27ClO2/c16-12-8-3-1-2-4-9-13-18-15(17)14-10-6-5-7-11-14/h14H,1-13H2
InchiKey:	TULIAZPVULJXOF-UHFFFAOYSA-N
Formula:	C15H27ClO2
SMILES:	O=C(OCCCCCCCCCl)C1CCCCC1
Mol. weight [g/mol]:	274.83

Physical Properties

Property code	Value	Unit	Source
gf	-145.98	kJ/mol	Joback Method
hf	-559.15	kJ/mol	Joback Method
hfus	33.42	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.689		Crippen Method
mvol	231.030	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2102.00		NIST Webbook
tb	675.87	K	Joback Method
tc	871.78	K	Joback Method
tf	368.27	K	Joback Method
vc	0.881	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/molxK	675.87	Joback Method
cpg	668.38	J/molxK	708.52	Joback Method
cpg	686.39	J/molxK	741.17	Joback Method
cpg	703.35	J/molxK	773.83	Joback Method
cpg	719.28	J/molxK	806.48	Joback Method
cpg	734.21	J/molxK	839.13	Joback Method
cpg	748.17	J/molxK	871.78	Joback Method
dvisc	0.0025138	Paxs	368.27	Joback Method
dvisc	0.0011386	Paxs	419.54	Joback Method

dvisc	0.0006128	Paxs	470.80	Joback Method
dvisc	0.0003725	Paxs	522.07	Joback Method
dvisc	0.0002475	Paxs	573.34	Joback Method
dvisc	0.0001759	Paxs	624.60	Joback Method
dvisc	0.0001316	Paxs	675.87	Joback Method

Sources

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=U354652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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