

Cyclohexanecarboxylic acid, octyl ester

Other names:	octyl cyclohexanecarboxylate
Inchi:	InChI=1S/C15H28O2/c1-2-3-4-5-6-10-13-17-15(16)14-11-8-7-9-12-14/h14H,2-13H2,1H3
InchiKey:	TZBMAJZGRONTGN-UHFFFAOYSA-N
Formula:	C15H28O2
SMILES:	CCCCCCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]:	240.38
CAS:	89611-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-134.05	kJ/mol	Joback Method
hf	-543.41	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.470		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1709.83		NIST Webbook
rinpol	1706.03		NIST Webbook
tb	638.44	K	Joback Method
tc	830.44	K	Joback Method
tf	338.35	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.82	J/molxK	638.44	Joback Method
cpg	635.04	J/molxK	670.44	Joback Method
cpg	654.20	J/molxK	702.44	Joback Method
cpg	672.33	J/molxK	734.44	Joback Method
cpg	689.44	J/molxK	766.44	Joback Method
cpg	705.57	J/molxK	798.44	Joback Method

cpg	720.72	J/mol×K	830.44	Joback Method
dvisc	0.0031539	Paxs	338.35	Joback Method
dvisc	0.0013572	Paxs	388.37	Joback Method
dvisc	0.0007079	Paxs	438.38	Joback Method
dvisc	0.0004219	Paxs	488.39	Joback Method
dvisc	0.0002768	Paxs	538.41	Joback Method
dvisc	0.0001951	Paxs	588.42	Joback Method
dvisc	0.0001453	Paxs	638.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89611201&Units=SI

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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