

Cyclopropanecarboxylic acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C12H21ClO2/c13-9-5-3-1-2-4-6-10-15-12(14)11-7-8-11/h11H,1-10H2
InchiKey:	KCXIAMVMCWDNHA-UHFFFAOYSA-N
Formula:	C12H21ClO2
SMILES:	O=C(OCCCCCCCCCl)C1CC1
Mol. weight [g/mol]:	232.75

Physical Properties

Property code	Value	Unit	Source
gf	-134.94	kJ/mol	Joback Method
hf	-478.75	kJ/mol	Joback Method
hfus	31.96	kJ/mol	Joback Method
hvap	55.76	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.519		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	594.42	K	Joback Method
tc	779.93	K	Joback Method
tf	345.02	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.46	J/molxK	594.42	Joback Method
cpg	552.90	J/molxK	749.01	Joback Method
cpg	540.25	J/molxK	718.09	Joback Method
cpg	526.92	J/molxK	687.18	Joback Method
cpg	512.86	J/molxK	656.26	Joback Method
cpg	498.05	J/molxK	625.34	Joback Method
cpg	564.89	J/molxK	779.93	Joback Method
dvisc	0.0004197	Paxs	594.42	Joback Method

dvisc	0.0005051	Paxs	552.85	Joback Method
dvisc	0.0006265	Paxs	511.29	Joback Method
dvisc	0.0008071	Paxs	469.72	Joback Method
dvisc	0.0010924	Paxs	428.15	Joback Method
dvisc	0.0015778	Paxs	386.59	Joback Method
dvisc	0.0024901	Paxs	345.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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