

Octanoic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C11H19ClO2/c1-2-3-4-5-6-8-11(13)14-10-7-9-12/h7,9H,2-6,8,10H2,1H3/b9-7+
InchiKey:	DQDAHPGZXVTTSA-VQHVLOKHSA-N
Formula:	C11H19ClO2
SMILES:	CCCCCCCC(=O)OCC=CCl
Mol. weight [g/mol]:	218.72

Physical Properties

Property code	Value	Unit	Source
gf	-123.89	kJ/mol	Joback Method
hf	-413.69	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	53.58	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.643		Crippen Method
mvol	181.230	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1468.00		NIST Webbook
tb	568.96	K	Joback Method
tc	751.82	K	Joback Method
tf	310.73	K	Joback Method
vc	0.705	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.48	J/molxK	568.96	Joback Method
cpg	441.43	J/molxK	599.44	Joback Method
cpg	454.74	J/molxK	629.91	Joback Method
cpg	467.42	J/molxK	660.39	Joback Method
cpg	479.49	J/molxK	690.86	Joback Method
cpg	490.98	J/molxK	721.34	Joback Method
cpg	501.90	J/molxK	751.82	Joback Method
dvisc	0.0025601	Paxs	310.73	Joback Method
dvisc	0.0012349	Paxs	353.77	Joback Method

dvisc	0.0006978	Paxs	396.81	Joback Method
dvisc	0.0004409	Paxs	439.85	Joback Method
dvisc	0.0003023	Paxs	482.88	Joback Method
dvisc	0.0002205	Paxs	525.92	Joback Method
dvisc	0.0001687	Paxs	568.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299350&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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