

2-chloroethyl tridecanoate

Inchi: InChI=1S/C15H29ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-15(17)18-14-13-16/h2-14H2,1H3
InchiKey: MWQGRPJKAJCUAN-UHFFFAOYSA-N
Formula: C15H29ClO2
SMILES: CCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 276.84

Physical Properties

Property code	Value	Unit	Source
gf	-170.43	kJ/mol	Joback Method
hf	-613.47	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.079		Crippen Method
mcvol	241.890	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
ripol	1896.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2383.00		NIST Webbook
ripol	2386.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2368.00		NIST Webbook
tb	656.32	K	Joback Method
tc	828.65	K	Joback Method
tf	360.89	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.00	J/molxK	656.32	Joback Method
cpg	731.03	J/molxK	799.93	Joback Method
cpg	717.25	J/molxK	771.21	Joback Method
cpg	702.78	J/molxK	742.49	Joback Method
cpg	687.59	J/molxK	713.76	Joback Method
cpg	671.67	J/molxK	685.04	Joback Method
cpg	744.13	J/molxK	828.65	Joback Method
dvisc	0.0001250	Paxs	656.32	Joback Method
dvisc	0.0001653	Paxs	607.08	Joback Method
dvisc	0.0002297	Paxs	557.84	Joback Method
dvisc	0.0003401	Paxs	508.60	Joback Method
dvisc	0.0005479	Paxs	459.37	Joback Method
dvisc	0.0009897	Paxs	410.13	Joback Method
dvisc	0.0021007	Paxs	360.89	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=R30880&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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