

Dichloroacetic acid, tetradecyl ester

Other names:	Tetradecyl dichloroacetate
Inchi:	InChI=1S/C16H30Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-16(19)15(17)18/h15H,2-
InchiKey:	JFGNOMDHPRPBJP-UHFFFAOYSA-N
Formula:	C16H30Cl2O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	325.31
CAS:	83005-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-176.38	kJ/mol	Joback Method
hf	-655.13	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.034		Crippen Method
mcvol	268.220	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2085.30		NIST Webbook
rinpol	2085.30		NIST Webbook
tb	716.19	K	Joback Method
tc	895.49	K	Joback Method
tf	387.08	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.82	J/molxK	716.19	Joback Method
cpg	760.33	J/molxK	746.07	Joback Method
cpg	776.01	J/molxK	775.96	Joback Method
cpg	790.89	J/molxK	805.84	Joback Method
cpg	804.98	J/molxK	835.72	Joback Method
cpg	818.31	J/molxK	865.61	Joback Method

cpg	830.90	J/mol×K	895.49	Joback Method
dvisc	0.0018889	Paxs	387.08	Joback Method
dvisc	0.0008297	Paxs	441.93	Joback Method
dvisc	0.0004370	Paxs	496.78	Joback Method
dvisc	0.0002615	Paxs	551.63	Joback Method
dvisc	0.0001717	Paxs	606.49	Joback Method
dvisc	0.0001209	Paxs	661.34	Joback Method
dvisc	0.0000898	Paxs	716.19	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=C83005021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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