Dichloroacetic acid, dodecyl ester

Other names: Dodecyl dichloroacetate
Inchi: InChI=1S/C14H26Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-18-14(17)13(15)16/h13H,2-12H2,1
InchiKey: XOWWGPRKFWEEDR-UHFFFAOYSA-N
Formula: C14H26Cl2O2
SMILES: CCCCCCCCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 297.26
CAS: 83005-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-193.22	kJ/mol	Joback Method
hf	-613.85	kJ/mol	Joback Method
hfus	39.67	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.254		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1884.80		NIST Webbook
rinpol	1884.80		NIST Webbook
tb	670.43	K	Joback Method
tc	850.28	K	Joback Method
tf	364.54	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.04	J/mol×K	670.43	Joback Method
cpg	703.85	J/mol×K	820.31	Joback Method
cpg	691.13	J/mol×K	790.33	Joback Method
cpg	677.72	J/mol×K	760.36	Joback Method
cpg	663.57	J/mol×K	730.38	Joback Method
cpg	648.69	J/mol×K	700.41	Joback Method

cpg	715.87	J/mol×K	850.28	Joback Method
dvisc	0.0001178	Pa×s	670.43	Joback Method
dvisc	0.0001578	Pa×s	619.45	Joback Method
dvisc	0.0002226	Pa×s	568.47	Joback Method
dvisc	0.0003361	Pa×s	517.49	Joback Method
dvisc	0.0005552	Pa×s	466.50	Joback Method
dvisc	0.0010376	Pa×s	415.52	Joback Method
dvisc	0.0023096	Pa×s	364.54	Joback Method

Sources

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=C83005010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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