Diethylmalonic acid, 2,2-dichloroethyl tetradecyl ester

Inchi: InChI=1S/C23H42Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-28-21(26)23(5-2,6-3)22
InchiKey: HKRLEKGIESRQBC-UHFFFAOYSA-N
Formula: C23H42Cl2O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 453.48

Physical Properties

Property code	Value	Unit	Source
gf	-348.52	kJ/mol	Joback Method
hf	-1053.16	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	92.19	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.384		Crippen Method
mcvol	374.290	ml/mol	McGowan Method
pc	874.80	kPa	Joback Method
rinpol	2723.00		NIST Webbook
tb	949.41	K	Joback Method
tc	1162.70	K	Joback Method
tf	540.55	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.06	J/mol×K	949.41	Joback Method
cpg	1289.79	J/mol×K	1127.16	Joback Method
cpg	1277.24	J/mol×K	1091.61	Joback Method
cpg	1263.55	J/mol×K	1056.06	Joback Method
cpg	1248.66	J/mol×K	1020.51	Joback Method
cpg	1232.52	J/mol×K	984.96	Joback Method
cpg	1301.27	J/mol×K	1162.70	Joback Method
dvisc	0.0000168	Pa×s	949.41	Joback Method
dvisc	0.0000230	Pa×s	881.27	Joback Method

dvisc	0.0000331	Pa×s	813.12	Joback Method
dvisc	0.0000509	Pa×s	744.98	Joback Method
dvisc	0.0000854	Pa×s	676.84	Joback Method
dvisc	0.0001610	Pa×s	608.69	Joback Method
dvisc	0.0003563	Pa×s	540.55	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=U370789&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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