Diethylmalonic acid, 2,2-dichloroethyl dodecyl ester

Inchi: InChI=1S/C21H38Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-26-19(24)21(5-2,6-3)20(25)27
InchiKey: FOOLFNHURAGYPE-UHFFFAOYSA-N
Formula: C21H38Cl2O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 425.43

Physical Properties

Property code	Value	Unit	Source
gf	-365.36	kJ/mol	Joback Method
hf	-1011.88	kJ/mol	Joback Method
hfus	53.18	kJ/mol	Joback Method
hvap	87.74	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.604		Crippen Method
mcvol	346.110	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	903.65	K	Joback Method
tc	1106.97	K	Joback Method
tf	518.01	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.95	J/mol×K	903.65	Joback Method
cpg	1164.06	J/mol×K	1073.08	Joback Method
cpg	1151.80	J/mol×K	1039.20	Joback Method
cpg	1138.50	J/mol×K	1005.31	Joback Method
cpg	1124.13	J/mol×K	971.42	Joback Method
cpg	1108.63	J/mol×K	937.54	Joback Method
cpg	1175.33	J/mol×K	1106.97	Joback Method
dvisc	0.0000234	Pa×s	903.65	Joback Method

dvisc	0.0000318	Pa×s	839.38	Joback Method
dvisc	0.0000456	Pa×s	775.10	Joback Method
dvisc	0.0000698	Pa×s	710.83	Joback Method
dvisc	0.0001162	Pa×s	646.56	Joback Method
dvisc	0.0002166	Pa×s	582.28	Joback Method
dvisc	0.0004710	Pa×s	518.01	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=U370787&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