Diethylmalonic acid, 2,2-dichloroethyl octyl ester

Inchi: InChI=1S/C17H30Cl2O4/c1-4-7-8-9-10-11-12-22-15(20)17(5-2,6-3)16(21)23-13-14(18)19

InchiKey: XWIFLEXPEUQYMP-UHFFFAOYSA-N

Formula: C17H30Cl2O4

SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 369.32

Physical Properties

Property code	Value	Unit	Source
gf	-399.04	kJ/mol	Joback Method
hf	-929.32	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	78.83	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.043		Crippen Method
mcvol	289.750	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	812.13	K	Joback Method
tc	1005.98	K	Joback Method
tf	472.93	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.73	J/mol×K	812.13	Joback Method
cpg	869.11	J/mol×K	844.44	Joback Method
cpg	883.50	J/mol×K	876.75	Joback Method
cpg	896.95	J/mol×K	909.06	Joback Method
cpg	909.48	J/mol×K	941.37	Joback Method
cpg	921.11	J/mol×K	973.67	Joback Method
cpg	931.89	J/mol×K	1005.98	Joback Method
dvisc	0.0007994	Pa×s	472.93	Joback Method

dvisc	0.0003822	Pa×s	529.46	Joback Method
dvisc	0.0002107	Pa×s	586.00	Joback Method
dvisc	0.0001290	Pa×s	642.53	Joback Method
dvisc	0.0000855	Pa×s	699.06	Joback Method
dvisc	0.0000602	Pa×s	755.60	Joback Method
dvisc	0.0000446	Pa×s	812.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U370783&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume