Diethylmalonic acid, 2,2-dichloroethyl propyl ester

Inchi: InChI=1S/C12H20Cl2O4/c1-4-7-17-10(15)12(5-2,6-3)11(16)18-8-9(13)14/h9H,4-8H2,1-3

InchiKey: CTXJBPOLAOHOQD-UHFFFAOYSA-N

Formula: C12H20Cl2O4

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

Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-441.14	kJ/mol	Joback Method
hf	-826.12	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	67.70	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.093		Crippen Method
mcvol	219.300	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	1627.00		NIST Webbook
tb	697.73	K	Joback Method
tc	894.59	K	Joback Method
tf	416.58	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.25	J/mol×K	697.73	Joback Method
cpg	636.08	J/mol×K	861.78	Joback Method
cpg	625.68	J/mol×K	828.97	Joback Method
cpg	614.51	J/mol×K	796.16	Joback Method
cpg	602.57	J/mol×K	763.35	Joback Method
cpg	589.82	J/mol×K	730.54	Joback Method
cpg	645.74	J/mol×K	894.59	Joback Method
dvisc	0.0000962	Pa×s	697.73	Joback Method
dvisc	0.0001284	Pa×s	650.87	Joback Method

dvisc	0.0001793	Pa×s	604.01	Joback Method
dvisc	0.0002646	Pa×s	557.15	Joback Method
dvisc	0.0004197	Pa×s	510.30	Joback Method
dvisc	0.0007306	Pa×s	463.44	Joback Method
dvisc	0.0014409	Pa×s	416.58	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=U370777&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

Latest version available from:
https://www.chemeo.com/cid/54-302-6/Diethylmalonic-acid-2-2-dichloroethyl-propyl-ester.pdf
Generated by Cheméo on 2024-10-12 05:56:21.137607687 +0000 UTC m=+3293443.774576936.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.