

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/molxK	697.73	Joback Method
cpg	589.82	J/molxK	730.54	Joback Method
cpg	602.57	J/molxK	763.35	Joback Method
cpg	614.51	J/molxK	796.16	Joback Method
cpg	625.68	J/molxK	828.97	Joback Method
cpg	636.08	J/molxK	861.78	Joback Method
cpg	645.74	J/molxK	894.59	Joback Method
dvisc	0.0014409	Paxs	416.58	Joback Method
dvisc	0.0007306	Paxs	463.44	Joback Method

dvisc	0.0004197	Paxs	510.30	Joback Method
dvisc	0.0002646	Paxs	557.15	Joback Method
dvisc	0.0001793	Paxs	604.01	Joback Method
dvisc	0.0001284	Paxs	650.87	Joback Method
dvisc	0.0000962	Paxs	697.73	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=U370777&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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