Diethylmalonic acid, ethyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H17Cl3O4/c1-4-10(5-2,8(15)17-6-3)9(16)18-7-11(12,13)14/h4-7H2,1-3H3
InchiKey: ICDBZPXXABQWIL-UHFFFAOYSA-N
Formula: C11H17Cl3O4
SMILES: CCOC(=O)C(CC)(CC)C(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 319.61

Physical Properties

Property code	Value	Unit	Source
gf	-456.21	kJ/mol	Joback Method
hf	-824.69	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.269		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	709.49	K	Joback Method
tc	918.24	K	Joback Method
tf	452.65	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.78	J/mol×K	709.49	Joback Method
cpg	563.95	J/mol×K	744.28	Joback Method
cpg	575.26	J/mol×K	779.07	Joback Method
cpg	585.75	J/mol×K	813.86	Joback Method
cpg	595.46	J/mol×K	848.66	Joback Method
cpg	604.42	J/mol×K	883.45	Joback Method
cpg	612.69	J/mol×K	918.24	Joback Method
dvisc	0.0010196	Pa×s	452.65	Joback Method
dvisc	0.0005666	Pa×s	495.46	Joback Method

dvisc	0.0003457	Pa×s	538.26	Joback Method
dvisc	0.0002269	Pa×s	581.07	Joback Method
dvisc	0.0001577	Pa×s	623.88	Joback Method
dvisc	0.0001149	Pa×s	666.68	Joback Method
dvisc	0.0000870	Pa×s	709.49	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=U370470&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