Diethylmalonic acid, 2,2-dichloroethyl ethyl ester

Inchi: InChI=1S/C11H18Cl2O4/c1-4-11(5-2,9(14)16-6-3)10(15)17-7-8(12)13/h8H,4-7H2,1-3H3
InchiKey: SKSSFYRJBAYHSG-UHFFFAOYSA-N
Formula: C11H18Cl2O4
SMILES: CCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 285.16

Physical Properties

Property code	Value	Unit	Source
gf	-449.56	kJ/mol	Joback Method
hf	-805.48	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.703		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	674.85	K	Joback Method
tc	873.79	K	Joback Method
tf	405.31	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.21	J/mol×K	674.85	Joback Method
cpg	537.29	J/mol×K	708.01	Joback Method
cpg	549.57	J/mol×K	741.16	Joback Method
cpg	561.09	J/mol×K	774.32	Joback Method
cpg	571.85	J/mol×K	807.47	Joback Method
cpg	581.88	J/mol×K	840.63	Joback Method
cpg	591.19	J/mol×K	873.79	Joback Method
dvisc	0.0016011	Pa×s	405.31	Joback Method

dvisc	0.0008229	Pa×s	450.23	Joback Method
dvisc	0.0004772	Pa×s	495.16	Joback Method
dvisc	0.0003030	Pa×s	540.08	Joback Method
dvisc	0.0002063	Pa×s	585.00	Joback Method
dvisc	0.0001484	Pa×s	629.93	Joback Method
dvisc	0.0001115	Pa×s	674.85	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=U370776&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