Diethylmalonic acid, monochloride, 2-methoxyethyl ester

Inchi: InChI=1S/C10H17ClO4/c1-4-10(5-2,8(11)12)9(13)15-7-6-14-3/h4-7H2,1-3H3
InchiKey: UPMSXHDZLSIVJZ-UHFFFAOYSA-N
Formula: C10H17ClO4
SMILES: CCC(CC)(C(=O)Cl)C(=O)OCCOC
Mol. weight [g/mol]: 236.69

Physical Properties

Property code	Value	Unit	Source
gf	-443.61	kJ/mol	Joback Method
hf	-763.82	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.748		Crippen Method
mcvol	178.880	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	614.98	K	Joback Method
tc	808.91	K	Joback Method
tf	379.12	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.78	J/mol×K	614.98	Joback Method
cpg	505.40	J/mol×K	776.59	Joback Method
cpg	495.02	J/mol×K	744.27	Joback Method
cpg	483.98	J/mol×K	711.95	Joback Method
cpg	472.27	J/mol×K	679.62	Joback Method
cpg	459.88	J/mol×K	647.30	Joback Method
cpg	515.12	J/mol×K	808.91	Joback Method
dvisc	0.0001563	Pa×s	614.98	Joback Method

dvisc	0.0002040	Pa×s	575.67	Joback Method
dvisc	0.0002769	Pa×s	536.36	Joback Method
dvisc	0.0003945	Pa×s	497.05	Joback Method
dvisc	0.0005973	Pa×s	457.74	Joback Method
dvisc	0.0009776	Pa×s	418.43	Joback Method
dvisc	0.0017721	Pa×s	379.12	Joback Method

Sources

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=U370686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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