Diethylmalonyl dichloride

Inchi: InChI=1S/C7H10Cl2O2/c1-3-7(4-2,5(8)10)6(9)11/h3-4H2,1-2H3
InchiKey: FWKCXFPQSXNCBW-UHFFFAOYSA-N
Formula: C7H10Cl2O2
SMILES: CCC(CC)(C(=O)Cl)C(=O)Cl
Mol. weight [g/mol]: 197.06
CAS: 54505-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-270.80	kJ/mol	Joback Method
hf	-453.20	kJ/mol	Joback Method
hfus	18.06	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.324		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1102.00		NIST Webbook
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tb	538.93	K	Joback Method
tc	749.59	K	Joback Method
tf	330.77	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.91	J/mol×K	538.93	Joback Method
cpg	296.22	J/mol×K	574.04	Joback Method
cpg	305.83	J/mol×K	609.15	Joback Method
cpg	314.78	J/mol×K	644.26	Joback Method
cpg	323.10	J/mol×K	679.37	Joback Method
cpg	330.83	J/mol×K	714.48	Joback Method
cpg	338.01	J/mol×K	749.59	Joback Method

dvisc	0.0037254	Pa×s	330.77	Joback Method
dvisc	0.0020714	Pa×s	365.46	Joback Method
dvisc	0.0012752	Pa×s	400.16	Joback Method
dvisc	0.0008482	Pa×s	434.85	Joback Method
dvisc	0.0005992	Pa×s	469.54	Joback Method
dvisc	0.0004440	Pa×s	504.24	Joback Method
dvisc	0.0003420	Pa×s	538.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54505725&Units=SI
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

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