Dimethylmalonyl chloride

Inchi: InChI=1S/C5H6Cl2O2/c1-5(2,3(6)8)4(7)9/h1-2H3
InchiKey: CJXQAYQWVNXIQE-UHFFFAOYSA-N
Formula: C5H6Cl2O2
SMILES: CC(C)(C(=O)Cl)C(=O)Cl
Mol. weight [g/mol]: 169.01
CAS: 5659-93-8

Physical Properties

Property code	Value	Unit	Source
gf	-287.64	kJ/mol	Joback Method
hf	-411.92	kJ/mol	Joback Method
hfus	12.88	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.543		Crippen Method
mcvol	108.930	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	915.30		NIST Webbook
tb	493.17	K	Joback Method
tc	710.74	K	Joback Method
tf	308.23	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.08	J/mol×K	493.17	Joback Method
cpg	211.19	J/mol×K	529.43	Joback Method
cpg	218.68	J/mol×K	565.69	Joback Method
cpg	225.59	J/mol×K	601.95	Joback Method
cpg	231.97	J/mol×K	638.21	Joback Method
cpg	237.83	J/mol×K	674.48	Joback Method
cpg	243.22	J/mol×K	710.74	Joback Method
dvisc	0.0040583	Pa×s	308.23	Joback Method

dvisc	0.0023470	Pa×s	339.05	Joback Method
dvisc	0.0014870	Pa×s	369.88	Joback Method
dvisc	0.0010106	Pa×s	400.70	Joback Method
dvisc	0.0007259	Pa×s	431.52	Joback Method
dvisc	0.0005448	Pa×s	462.35	Joback Method
dvisc	0.0004239	Pa×s	493.17	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=C5659938&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