

Dimethyl chloromalonate

Inchi:	InChI=1S/C5H7ClO4/c1-9-4(7)3(6)5(8)10-2/h3H,1-2H3
InchiKey:	LNBQBURECUEBKZ-UHFFFAOYSA-N
Formula:	C5H7ClO4
SMILES:	COC(=O)C(Cl)C(=O)OC
Mol. weight [g/mol]:	166.56
CAS:	28868-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-490.99	kJ/mol	Joback Method
hf	-657.15	kJ/mol	Joback Method
hfus	14.95	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	-0.060		Crippen Method
mcvol	108.430	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1018.00		NIST Webbook
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tb	503.37	K	Joback Method
tc	703.22	K	Joback Method
tf	305.35	K	Joback Method
vc	0.406	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.70	J/mol×K	503.37	Joback Method
cpg	255.49	J/mol×K	669.91	Joback Method
cpg	248.76	J/mol×K	636.60	Joback Method
cpg	241.70	J/mol×K	603.29	Joback Method
cpg	234.32	J/mol×K	569.99	Joback Method
cpg	226.65	J/mol×K	536.68	Joback Method
cpg	261.88	J/mol×K	703.22	Joback Method

dvisc	0.0002766	Paxs	503.37	Joback Method
dvisc	0.0003519	Paxs	470.37	Joback Method
dvisc	0.0004642	Paxs	437.36	Joback Method
dvisc	0.0006408	Paxs	404.36	Joback Method
dvisc	0.0009366	Paxs	371.36	Joback Method
dvisc	0.0014741	Paxs	338.35	Joback Method
dvisc	0.0025593	Paxs	305.35	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=C28868760&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
mvol:	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

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