

Dimethylmalonic acid, 4-chlorophenyl ethyl ester

Inchi:	InChI=1S/C13H15ClO4/c1-4-17-11(15)13(2,3)12(16)18-10-7-5-9(14)6-8-10/h5-8H,4H2,1
InchiKey:	YARLDFPKAPGMBN-UHFFFAOYSA-N
Formula:	C13H15ClO4
SMILES:	CCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	270.71

Physical Properties

Property code	Value	Unit	Source
gf	-315.57	kJ/mol	Joback Method
hf	-600.68	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.835		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinsol	1727.00		NIST Webbook
tb	715.28	K	Joback Method
tc	938.11	K	Joback Method
tf	451.87	K	Joback Method
vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.80	J/molxK	715.28	Joback Method
cpg	529.03	J/molxK	752.42	Joback Method
cpg	541.26	J/molxK	789.56	Joback Method
cpg	552.53	J/molxK	826.69	Joback Method
cpg	562.86	J/molxK	863.83	Joback Method
cpg	572.28	J/molxK	900.97	Joback Method
cpg	580.84	J/molxK	938.11	Joback Method
dvisc	0.0008920	Paxs	451.87	Joback Method
dvisc	0.0005291	Paxs	495.77	Joback Method

dvisc	0.0003417	Paxs	539.67	Joback Method
dvisc	0.0002357	Paxs	583.58	Joback Method
dvisc	0.0001712	Paxs	627.48	Joback Method
dvisc	0.0001297	Paxs	671.38	Joback Method
dvisc	0.0001016	Paxs	715.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361970&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

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