

Dimethylmalonic acid, monochloride, 2-methylphenyl ester

Inchi:	InChI=1S/C12H13ClO3/c1-8-6-4-5-7-9(8)16-11(15)12(2,3)10(13)14/h4-7H,1-3H3
InchiKey:	OPAZIZANYHYINM-UHFFFAOYSA-N
Formula:	C12H13ClO3
SMILES:	Cc1ccccc1OC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	240.68

Physical Properties

Property code	Value	Unit	Source
gf	-218.99	kJ/mol	Joback Method
hf	-447.82	kJ/mol	Joback Method
hfus	21.66	kJ/mol	Joback Method
hvap	64.23	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.692		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinsol	1555.00		NIST Webbook
tb	669.98	K	Joback Method
tc	899.84	K	Joback Method
tf	418.37	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.88	J/molxK	669.98	Joback Method
cpg	495.68	J/molxK	861.53	Joback Method
cpg	486.32	J/molxK	823.22	Joback Method
cpg	476.11	J/molxK	784.91	Joback Method
cpg	465.00	J/molxK	746.60	Joback Method
cpg	452.94	J/molxK	708.29	Joback Method
cpg	504.23	J/molxK	899.84	Joback Method
dvisc	0.0001511	Paxs	669.98	Joback Method
dvisc	0.0001929	Paxs	628.05	Joback Method

dvisc	0.0002550	Paxs	586.11	Joback Method
dvisc	0.0003518	Paxs	544.17	Joback Method
dvisc	0.0005123	Paxs	502.24	Joback Method
dvisc	0.0007988	Paxs	460.31	Joback Method
dvisc	0.0013615	Paxs	418.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361913&Units=SI
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

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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