

Dimethylmalonic acid, monochloride, 2-ethylphenyl ester

Inchi:	InChI=1S/C13H15ClO3/c1-4-9-7-5-6-8-10(9)17-12(16)13(2,3)11(14)15/h5-8H,4H2,1-3H3
InchiKey:	ULZVSXQZZSBOJD-UHFFFAOYSA-N
Formula:	C13H15ClO3
SMILES:	CCc1ccccc1OC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	254.71

Physical Properties

Property code	Value	Unit	Source
gf	-210.57	kJ/mol	Joback Method
hf	-468.46	kJ/mol	Joback Method
hfus	24.25	kJ/mol	Joback Method
hvap	66.46	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.946		Crippen Method
mcvol	191.520	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinsol	1683.00		NIST Webbook
tb	692.86	K	Joback Method
tc	918.48	K	Joback Method
tf	429.64	K	Joback Method
vc	0.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.56	J/molxK	692.86	Joback Method
cpg	504.13	J/molxK	730.46	Joback Method
cpg	516.69	J/molxK	768.07	Joback Method
cpg	528.29	J/molxK	805.67	Joback Method
cpg	538.98	J/molxK	843.27	Joback Method
cpg	548.79	J/molxK	880.88	Joback Method
cpg	557.79	J/molxK	918.48	Joback Method
dvisc	0.0012609	Paxs	429.64	Joback Method
dvisc	0.0007287	Paxs	473.51	Joback Method

dvisc	0.0004621	Paxs	517.38	Joback Method
dvisc	0.0003147	Paxs	561.25	Joback Method
dvisc	0.0002266	Paxs	605.12	Joback Method
dvisc	0.0001706	Paxs	648.99	Joback Method
dvisc	0.0001331	Paxs	692.86	Joback Method

Sources

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=U363854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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