

Dimethylmalonic acid, ethyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O4/c1-4-19-11(17)13(2,3)12(18)20-10-8(15)5-7(14)6-9(10)16/h5-6H
InchiKey:	VMYHHAPFJCPJOM-UHFFFAOYSA-N
Formula:	C13H13Cl3O4
SMILES:	CCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	339.60

Physical Properties

Property code	Value	Unit	Source
gf	-358.69	kJ/mol	Joback Method
hf	-655.10	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.141		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1998.00		NIST Webbook
tb	800.10	K	Joback Method
tc	1029.93	K	Joback Method
tf	536.75	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.03	J/mol×K	800.10	Joback Method
cpg	568.73	J/mol×K	838.41	Joback Method
cpg	578.47	J/mol×K	876.71	Joback Method
cpg	587.29	J/mol×K	915.02	Joback Method
cpg	595.22	J/mol×K	953.32	Joback Method
cpg	602.26	J/mol×K	991.63	Joback Method
cpg	608.44	J/mol×K	1029.93	Joback Method
dvisc	0.0004617	Paxs	536.75	Joback Method
dvisc	0.0003067	Paxs	580.64	Joback Method

dvisc	0.0002157	Paxs	624.53	Joback Method
dvisc	0.0001590	Paxs	668.42	Joback Method
dvisc	0.0001216	Paxs	712.32	Joback Method
dvisc	0.0000960	Paxs	756.21	Joback Method
dvisc	0.0000777	Paxs	800.10	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=U363644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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