

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

Inchi:	InChI=1S/C15H17Cl3O4/c1-8(2)7-21-13(19)15(3,4)14(20)22-12-10(17)5-9(16)6-11(12)18
InchiKey:	FFIVIPHUOGITAI-UHFFFAOYSA-N
Formula:	C15H17Cl3O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	367.65

Physical Properties

Property code	Value	Unit	Source
gf	-344.29	kJ/mol	Joback Method
hf	-701.66	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.778		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinsol	2133.00		NIST Webbook
tb	845.42	K	Joback Method
tc	1072.72	K	Joback Method
tf	544.29	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.74	J/molxK	845.42	Joback Method
cpg	714.30	J/molxK	1034.84	Joback Method
cpg	706.76	J/molxK	996.95	Joback Method
cpg	698.26	J/molxK	959.07	Joback Method
cpg	688.78	J/molxK	921.19	Joback Method
cpg	678.28	J/molxK	883.30	Joback Method
cpg	720.91	J/molxK	1072.72	Joback Method
dvisc	0.0000532	Paxs	845.42	Joback Method
dvisc	0.0000672	Paxs	795.23	Joback Method

dvisc	0.0000876	Paxs	745.04	Joback Method
dvisc	0.0001186	Paxs	694.86	Joback Method
dvisc	0.0001685	Paxs	644.67	Joback Method
dvisc	0.0002539	Paxs	594.48	Joback Method
dvisc	0.0004127	Paxs	544.29	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=U363646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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