

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

Inchi:	InChI=1S/C17H21Cl3O4/c1-10(2)6-5-7-23-15(21)17(3,4)16(22)24-14-12(19)8-11(18)9-13
InchiKey:	NESQWCKSIZSKSL-UHFFFAOYSA-N
Formula:	C17H21Cl3O4
SMILES:	CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	395.70

Physical Properties

Property code	Value	Unit	Source
gf	-327.45	kJ/mol	Joback Method
hf	-742.94	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.558		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2318.00		NIST Webbook
tb	891.18	K	Joback Method
tc	1114.69	K	Joback Method
tf	566.83	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.49	J/molxK	891.18	Joback Method
cpg	790.52	J/molxK	928.43	Joback Method
cpg	801.45	J/molxK	965.68	Joback Method
cpg	811.32	J/molxK	1002.93	Joback Method
cpg	820.17	J/molxK	1040.19	Joback Method
cpg	828.03	J/molxK	1077.44	Joback Method
cpg	834.93	J/molxK	1114.69	Joback Method
dvisc	0.0003309	Paxs	566.83	Joback Method
dvisc	0.0001987	Paxs	620.89	Joback Method

dvisc	0.0001295	Paxs	674.95	Joback Method
dvisc	0.0000899	Paxs	729.00	Joback Method
dvisc	0.0000657	Paxs	783.06	Joback Method
dvisc	0.0000499	Paxs	837.12	Joback Method
dvisc	0.0000393	Paxs	891.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363649&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

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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