

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

Inchi:	InChI=1S/C17H21Cl3O4/c1-4-5-6-7-8-23-15(21)17(2,3)16(22)24-14-12(19)9-11(18)10-13
InchiKey:	DYHDIIFPSIMVPV-UHFFFAOYSA-N
Formula:	C17H21Cl3O4
SMILES:	CCCCCOC(=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	-325.01	kJ/mol	Joback Method
hf	-737.66	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.702		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinsol	2359.00		NIST Webbook
tb	891.62	K	Joback Method
tc	1112.64	K	Joback Method
tf	581.83	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.94	J/molxK	891.62	Joback Method
cpg	827.34	J/molxK	1075.80	Joback Method
cpg	819.44	J/molxK	1038.97	Joback Method
cpg	810.59	J/molxK	1002.13	Joback Method
cpg	800.74	J/molxK	965.29	Joback Method
cpg	789.87	J/molxK	928.46	Joback Method
cpg	834.32	J/molxK	1112.64	Joback Method
dvisc	0.0000429	Paxs	891.62	Joback Method
dvisc	0.0000539	Paxs	839.99	Joback Method

dvisc	0.0000696	Paxs	788.36	Joback Method
dvisc	0.0000931	Paxs	736.72	Joback Method
dvisc	0.0001303	Paxs	685.09	Joback Method
dvisc	0.0001925	Paxs	633.46	Joback Method
dvisc	0.0003048	Paxs	581.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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