

Dimethylmalonic acid, 4-chlorophenyl isohehexyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-12(2)6-5-11-21-15(19)17(3,4)16(20)22-14-9-7-13(18)8-10-14/
InchiKey:	OGHCFELJQDDNJR-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-284.33	kJ/mol	Joback Method
hf	-688.52	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.251		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2056.00		NIST Webbook
tb	806.36	K	Joback Method
tc	1021.16	K	Joback Method
tf	481.95	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.48	J/molxK	806.36	Joback Method
cpg	796.13	J/molxK	985.36	Joback Method
cpg	785.68	J/molxK	949.56	Joback Method
cpg	774.22	J/molxK	913.76	Joback Method
cpg	761.73	J/molxK	877.96	Joback Method
cpg	748.16	J/molxK	842.16	Joback Method
cpg	805.62	J/molxK	1021.16	Joback Method
dvisc	0.0000531	Paxs	806.36	Joback Method
dvisc	0.0000699	Paxs	752.29	Joback Method

dvisc	0.0000960	Paxs	698.22	Joback Method
dvisc	0.0001390	Paxs	644.15	Joback Method
dvisc	0.0002155	Paxs	590.09	Joback Method
dvisc	0.0003647	Paxs	536.02	Joback Method
dvisc	0.0006949	Paxs	481.95	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361975&Units=SI

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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