

Dimethylmalonic acid, 4-chlorophenyl pentyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-4-5-6-11-20-14(18)16(2,3)15(19)21-13-9-7-12(17)8-10-13/h7-
InchiKey:	IEXKTFQLGHCIEU-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-290.31	kJ/mol	Joback Method
hf	-662.60	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.005		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	783.92	K	Joback Method
tc	997.75	K	Joback Method
tf	485.68	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.07	J/molxK	783.92	Joback Method
cpg	691.32	J/molxK	819.56	Joback Method
cpg	704.51	J/molxK	855.20	Joback Method
cpg	716.69	J/molxK	890.83	Joback Method
cpg	727.87	J/molxK	926.47	Joback Method
cpg	738.11	J/molxK	962.11	Joback Method
cpg	747.43	J/molxK	997.75	Joback Method
dvisc	0.0006732	Paxs	485.68	Joback Method

dvisc	0.0003832	Paxs	535.39	Joback Method
dvisc	0.0002400	Paxs	585.09	Joback Method
dvisc	0.0001618	Paxs	634.80	Joback Method
dvisc	0.0001155	Paxs	684.51	Joback Method
dvisc	0.0000863	Paxs	734.21	Joback Method
dvisc	0.0000669	Paxs	783.92	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=U361974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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