

Diethylmalonic acid, monochloride, 3-methoxyphenyl ester

Inchi:	InChI=1S/C14H17ClO4/c1-4-14(5-2,12(15)16)13(17)19-11-8-6-7-10(9-11)18-3/h6-9H,4-5
InchiKey:	AMFOIQKDNQFXOS-UHFFFAOYSA-N
Formula:	C14H17ClO4
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1cccc(OC)c1
Mol. weight [g/mol]:	284.74

Physical Properties

Property code	Value	Unit	Source
gf	-307.15	kJ/mol	Joback Method
hf	-621.32	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.172		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1908.00		NIST Webbook
tb	738.16	K	Joback Method
tc	957.50	K	Joback Method
tf	463.14	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.43	J/molxK	738.16	Joback Method
cpg	626.73	J/molxK	920.94	Joback Method
cpg	616.98	J/molxK	884.39	Joback Method
cpg	606.30	J/molxK	847.83	Joback Method
cpg	594.68	J/molxK	811.27	Joback Method
cpg	582.06	J/molxK	774.72	Joback Method
cpg	635.59	J/molxK	957.50	Joback Method
dvisc	0.0000887	Paxs	738.16	Joback Method
dvisc	0.0001136	Paxs	692.32	Joback Method

dvisc	0.0001507	Paxs	646.49	Joback Method
dvisc	0.0002087	Paxs	600.65	Joback Method
dvisc	0.0003050	Paxs	554.81	Joback Method
dvisc	0.0004774	Paxs	508.98	Joback Method
dvisc	0.0008163	Paxs	463.14	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=U370878&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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