

Diethylmalonic acid, monochloride, 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C14H16Cl2O3/c1-4-14(5-2,12(16)17)13(18)19-11-7-6-10(15)8-9(11)3/h6-8H,4
InchiKey:	LSPYBBRTGROWTB-UHFFFAOYSA-N
Formula:	C14H16Cl2O3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	303.18

Physical Properties

Property code	Value	Unit	Source
gf	-223.71	kJ/mol	Joback Method
hf	-516.31	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.126		Crippen Method
mcvol	217.850	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinsol	1930.00		NIST Webbook
tb	758.15	K	Joback Method
tc	983.54	K	Joback Method
tf	483.35	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.62	J/molxK	758.15	Joback Method
cpg	619.85	J/molxK	945.97	Joback Method
cpg	610.76	J/molxK	908.41	Joback Method
cpg	600.85	J/molxK	870.84	Joback Method
cpg	590.05	J/molxK	833.28	Joback Method
cpg	578.32	J/molxK	795.71	Joback Method
cpg	628.14	J/molxK	983.54	Joback Method
dvisc	0.0001028	Paxs	758.15	Joback Method
dvisc	0.0001299	Paxs	712.35	Joback Method

dvisc	0.0001694	Paxs	666.55	Joback Method
dvisc	0.0002299	Paxs	620.75	Joback Method
dvisc	0.0003275	Paxs	574.95	Joback Method
dvisc	0.0004960	Paxs	529.15	Joback Method
dvisc	0.0008126	Paxs	483.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370123&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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