Diethylmalonic acid, monochloride, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C15H19ClO3/c1-5-15(6-2,13(16)17)14(18)19-12-9-7-8-10(3)11(12)4/h7-9H,5-6

InchiKey: MCROHUZXPLHPEK-UHFFFAOYSA-N

Formula: C15H19ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 282.76

Physical Properties

Property code	Value	Unit	Source
gf	-203.36	kJ/mol	Joback Method
hf	-521.21	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.781		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1883.00		NIST Webbook
tb	743.60	K	Joback Method
tc	962.75	K	Joback Method
tf	464.70	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.63	J/mol×K	743.60	Joback Method
cpg	608.88	J/mol×K	780.13	Joback Method
cpg	622.13	J/mol×K	816.65	Joback Method
cpg	634.40	J/mol×K	853.18	Joback Method
cpg	645.75	J/mol×K	889.70	Joback Method
cpg	656.22	J/mol×K	926.23	Joback Method
cpg	665.85	J/mol×K	962.75	Joback Method
dvisc	0.0008875	Pa×s	464.70	Joback Method
dvisc	0.0005253	Pa×s	511.18	Joback Method

dvisc	0.0003393	Pa×s	557.67	Joback Method
dvisc	0.0002344	Pa×s	604.15	Joback Method
dvisc	0.0001708	Pa×s	650.63	Joback Method
dvisc	0.0001298	Pa×s	697.12	Joback Method
dvisc	0.0001020	Pa×s	743.60	Joback Method

Sources

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=U370581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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