Diethylmalonic acid, monochloride, 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C15H19ClO5/c1-5-15(6-2,13(16)17)14(18)21-12-10(19-3)8-7-9-11(12)20-4/h7-

InchiKey: SPKLDHKFKUDGKF-UHFFFAOYSA-N

Formula: C15H19ClO5

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 314.76

Physical Properties

Property code	Value	Unit	Source
gf	-413.36	kJ/mol	Joback Method
hf	-785.65	kJ/mol	Joback Method
hfus	31.41	kJ/mol	Joback Method
hvap	76.39	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.181		Crippen Method
mcvol	231.440	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2084.00		NIST Webbook
tb	788.44	K	Joback Method
tc	1003.86	K	Joback Method
tf	509.16	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.61	J/mol×K	788.44	Joback Method
cpg	661.06	J/mol×K	824.34	Joback Method
cpg	673.45	J/mol×K	860.25	Joback Method
cpg	684.80	J/mol×K	896.15	Joback Method
cpg	695.12	J/mol×K	932.05	Joback Method
cpg	704.41	J/mol×K	967.96	Joback Method
cpg	712.71	J/mol×K	1003.86	Joback Method
dvisc	0.0004457	Pa×s	509.16	Joback Method
dvisc	0.0002755	Pa×s	555.71	Joback Method

dvisc	0.0001834	Pa×s	602.25	Joback Method
dvisc	0.0001295	Pa×s	648.80	Joback Method
dvisc	0.0000958	Pa×s	695.35	Joback Method
dvisc	0.0000735	Pa×s	741.89	Joback Method
dvisc	0.0000583	Pa×s	788.44	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=U369819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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