Diethylmalonic acid, monochloride, 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C13H12Cl4O3/c1-3-13(4-2,11(17)18)12(19)20-10-8(15)5-7(14)6-9(10)16/h5-6H

InchiKey: LWSJBUSTUXCWLM-UHFFFAOYSA-N

Formula: C13H12Cl4O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 358.05

Physical Properties

Property code	Value	Unit	Source
gf	-265.62	kJ/mol	Joback Method
hf	-538.62	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.124		Crippen Method
mcvol	228.240	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	815.11	K	Joback Method
tc	1050.07	K	Joback Method
tf	544.44	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.02	J/mol×K	815.11	Joback Method
cpg	595.24	J/mol×K	1010.91	Joback Method
cpg	588.57	J/mol×K	971.75	Joback Method
cpg	581.16	J/mol×K	932.59	Joback Method
cpg	572.96	J/mol×K	893.43	Joback Method
cpg	563.93	J/mol×K	854.27	Joback Method
cpg	601.21	J/mol×K	1050.07	Joback Method
dvisc	0.0000893	Pa×s	815.11	Joback Method

dvisc	0.0001104	Pa×s	770.00	Joback Method
dvisc	0.0001402	Pa×s	724.89	Joback Method
dvisc	0.0001837	Pa×s	679.77	Joback Method
dvisc	0.0002502	Pa×s	634.66	Joback Method
dvisc	0.0003573	Pa×s	589.55	Joback Method
dvisc	0.0005412	Pa×s	544.44	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=U370158&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