Diethylmalonic acid, isobutyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C17H21Cl3O4/c1-5-17(6-2,15(21)23-9-10(3)4)16(22)24-14-12(19)8-7-11(18)13

InchiKey: QZTXOSYZSUHOQZ-UHFFFAOYSA-N

Formula: C17H21Cl3O4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 395.70

Physical Properties

Property code	Value	Unit	Source
gf	-327.45	kJ/mol	Joback Method
hf	-742.94	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.558		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2373.00		NIST Webbook
tb	891.18	K	Joback Method
tc	1114.69	K	Joback Method
tf	566.83	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.49	J/mol×K	891.18	Joback Method
cpg	828.03	J/mol×K	1077.44	Joback Method
cpg	820.17	J/mol×K	1040.19	Joback Method
cpg	811.32	J/mol×K	1002.93	Joback Method
cpg	801.45	J/mol×K	965.68	Joback Method
cpg	790.52	J/mol×K	928.43	Joback Method
cpg	834.93	J/mol×K	1114.69	Joback Method
dvisc	0.0000393	Pa×s	891.18	Joback Method
dvisc	0.0000499	Pa×s	837.12	Joback Method

dvisc	0.0000657	Pa×s	783.06	Joback Method
dvisc	0.0000899	Pa×s	729.00	Joback Method
dvisc	0.0001295	Pa×s	674.95	Joback Method
dvisc	0.0001987	Pa×s	620.89	Joback Method
dvisc	0.0003309	Pa×s	566.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370283&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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