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

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

InchiKey: OROBCZUVINWAJN-UHFFFAOYSA-N

Formula: C17H21Cl3O4

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

Mol. weight [g/mol]: 395.70

Physical Properties

Property code	Value	Unit	Source
gf	-325.01	kJ/mol	Joback Method
hf	-737.66	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.702		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	891.62	K	Joback Method
tc	1112.64	K	Joback Method
tf	581.83	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.94	J/mol×K	891.62	Joback Method
cpg	827.34	J/mol×K	1075.80	Joback Method
cpg	819.44	J/mol×K	1038.97	Joback Method
cpg	810.59	J/mol×K	1002.13	Joback Method
cpg	800.74	J/mol×K	965.29	Joback Method
cpg	789.87	J/mol×K	928.46	Joback Method
cpg	834.32	J/mol×K	1112.64	Joback Method
dvisc	0.0000429	Pa×s	891.62	Joback Method

dvisc	0.0000539	Pa×s	839.99	Joback Method
dvisc	0.0000696	Pa×s	788.36	Joback Method
dvisc	0.0000931	Pa×s	736.72	Joback Method
dvisc	0.0001303	Pa×s	685.09	Joback Method
dvisc	0.0001925	Pa×s	633.46	Joback Method
dvisc	0.0003048	Pa×s	581.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370284&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

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