Diethylmalonic acid, 2-chlorophenyl isobutyl ester

Inchi: InChI=1S/C17H23ClO4/c1-5-17(6-2,15(19)21-11-12(3)4)16(20)22-14-10-8-7-9-13(14)18/

InchiKey: AYEPGUHGRUONBS-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-284.33	kJ/mol	Joback Method
hf	-688.52	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.251		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2023.00		NIST Webbook
tb	806.36	K	Joback Method
tc	1021.16	K	Joback Method
tf	481.95	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.48	J/mol×K	806.36	Joback Method
cpg	796.13	J/mol×K	985.36	Joback Method
cpg	785.68	J/mol×K	949.56	Joback Method
cpg	774.22	J/mol×K	913.76	Joback Method
cpg	761.73	J/mol×K	877.96	Joback Method
cpg	748.16	J/mol×K	842.16	Joback Method
cpg	805.62	J/mol×K	1021.16	Joback Method
dvisc	0.0000531	Pa×s	806.36	Joback Method
dvisc	0.0000699	Pa×s	752.29	Joback Method

dvisc	0.0000960	Pa×s	698.22	Joback Method
dvisc	0.0001390	Pa×s	644.15	Joback Method
dvisc	0.0002155	Pa×s	590.09	Joback Method
dvisc	0.0003647	Pa×s	536.02	Joback Method
dvisc	0.0006949	Pa×s	481.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369614&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