Diethylmalonic acid, 2-chloro-5-methylphenyl propyl ester

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

InchiKey: RGBOIGQCAGMDGV-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-291.52	kJ/mol	Joback Method
hf	-694.71	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.313		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	811.78	K	Joback Method
tc	1024.45	K	Joback Method
tf	509.47	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.90	J/mol×K	811.78	Joback Method
cpg	793.54	J/mol×K	989.00	Joback Method
cpg	783.22	J/mol×K	953.56	Joback Method
cpg	771.93	J/mol×K	918.11	Joback Method
cpg	759.64	J/mol×K	882.67	Joback Method
cpg	746.30	J/mol×K	847.22	Joback Method
cpg	802.91	J/mol×K	1024.45	Joback Method
dvisc	0.0000583	Pa×s	811.78	Joback Method

dvisc	0.0000744	Pa×s	761.39	Joback Method
dvisc	0.0000983	Pa×s	711.01	Joback Method
dvisc	0.0001355	Pa×s	660.62	Joback Method
dvisc	0.0001968	Pa×s	610.24	Joback Method
dvisc	0.0003060	Pa×s	559.86	Joback Method
dvisc	0.0005189	Pa×s	509.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370452&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