Diethylmalonic acid, 2-chlorophenyl propyl ester

Inchi: InChI=1S/C16H21ClO4/c1-4-11-20-14(18)16(5-2,6-3)15(19)21-13-10-8-7-9-12(13)17/h7-

InchiKey: NHGYTQNAPZFWFZ-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-290.31	kJ/mol	Joback Method
hf	-662.60	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.005		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	783.92	K	Joback Method
tc	997.75	K	Joback Method
tf	485.68	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.07	J/mol×K	783.92	Joback Method
cpg	691.32	J/mol×K	819.56	Joback Method
cpg	704.51	J/mol×K	855.20	Joback Method
cpg	716.69	J/mol×K	890.83	Joback Method
cpg	727.87	J/mol×K	926.47	Joback Method
cpg	738.11	J/mol×K	962.11	Joback Method
cpg	747.43	J/mol×K	997.75	Joback Method
dvisc	0.0006732	Pa×s	485.68	Joback Method

dvisc	0.0003832	Pa×s	535.39	Joback Method
dvisc	0.0002400	Pa×s	585.09	Joback Method
dvisc	0.0001618	Pa×s	634.80	Joback Method
dvisc	0.0001155	Pa×s	684.51	Joback Method
dvisc	0.0000863	Pa×s	734.21	Joback Method
dvisc	0.0000669	Pa×s	783.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369613&Units=SI

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