Diethylmalonic acid, 4-chlorophenyl ethyl ester

Inchi: InChI=1S/C15H19ClO4/c1-4-15(5-2,13(17)19-6-3)14(18)20-12-9-7-11(16)8-10-12/h7-10H

InchiKey: RMBSYOLXIBKWOZ-UHFFFAOYSA-N

Formula: C15H19ClO4

SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-298.73	kJ/mol	Joback Method
hf	-641.96	kJ/mol	Joback Method
hfus	30.62	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.615		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	761.04	K	Joback Method
tc	977.37	K	Joback Method
tf	474.41	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.21	J/mol×K	761.04	Joback Method
cpg	636.18	J/mol×K	797.09	Joback Method
cpg	649.11	J/mol×K	833.15	Joback Method
cpg	661.04	J/mol×K	869.20	Joback Method
cpg	671.99	J/mol×K	905.26	Joback Method
cpg	682.01	J/mol×K	941.31	Joback Method
cpg	691.13	J/mol×K	977.37	Joback Method
dvisc	0.0007431	Pa×s	474.41	Joback Method

dvisc	0.0004286	Pa×s	522.18	Joback Method
dvisc	0.0002711	Pa×s	569.95	Joback Method
dvisc	0.0001841	Pa×s	617.73	Joback Method
dvisc	0.0001321	Pa×s	665.50	Joback Method
dvisc	0.0000992	Pa×s	713.27	Joback Method
dvisc	0.0000771	Pa×s	761.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369891&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