Diethylmalonic acid, butyl 4-chloro-2-methylphenyl ester

Inchi: InChI=1S/C18H25ClO4/c1-5-8-11-22-16(20)18(6-2,7-3)17(21)23-15-10-9-14(19)12-13(15

InchiKey: SLMRDCQRRMCCFM-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-283.10	kJ/mol	Joback Method
hf	-715.35	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.704		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	834.66	K	Joback Method
tc	1046.00	K	Joback Method
tf	520.74	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.73	J/mol×K	834.66	Joback Method
cpg	803.35	J/mol×K	869.88	Joback Method
cpg	816.87	J/mol×K	905.11	Joback Method
cpg	829.34	J/mol×K	940.33	Joback Method
cpg	840.78	J/mol×K	975.55	Joback Method
cpg	851.23	J/mol×K	1010.78	Joback Method
cpg	860.72	J/mol×K	1046.00	Joback Method
dvisc	0.0004680	Pa×s	520.74	Joback Method

dvisc	0.0002725	Pa×s	573.06	Joback Method
dvisc	0.0001737	Pa×s	625.38	Joback Method
dvisc	0.0001187	Pa×s	677.70	Joback Method
dvisc	0.0000857	Pa×s	730.02	Joback Method
dvisc	0.0000646	Pa×s	782.34	Joback Method
dvisc	0.0000504	Pa×s	834.66	Joback Method

Sources

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=U370108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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