Diethylmalonic acid, 3-chlorobenzyl propyl ester

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

InchiKey: IAACNAUBBBRQRJ-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-281.89	kJ/mol	Joback Method
hf	-683.24	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.143		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	806.80	K	Joback Method
tc	1018.69	K	Joback Method
tf	496.95	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.92	J/mol×K	806.80	Joback Method
cpg	795.00	J/mol×K	983.37	Joback Method
cpg	784.59	J/mol×K	948.06	Joback Method
cpg	773.21	J/mol×K	912.74	Joback Method
cpg	760.83	J/mol×K	877.43	Joback Method
cpg	747.41	J/mol×K	842.11	Joback Method
cpg	804.50	J/mol×K	1018.69	Joback Method
dvisc	0.0000579	Pa×s	806.80	Joback Method

dvisc	0.0000749	Pa×s	755.16	Joback Method
dvisc	0.0001006	Pa×s	703.52	Joback Method
dvisc	0.0001417	Pa×s	651.88	Joback Method
dvisc	0.0002118	Pa×s	600.23	Joback Method
dvisc	0.0003412	Pa×s	548.59	Joback Method
dvisc	0.0006071	Pa×s	496.95	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=U369342&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