

Diethylmalonic acid, butyl 3,5-dichlorophenyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-4-7-8-22-15(20)17(5-2,6-3)16(21)23-14-10-12(18)9-13(19)1
InchiKey:	ZZMAGLZYMIRBIA-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-303.45	kJ/mol	Joback Method
hf	-710.45	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	82.82	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.048		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2160.00		NIST Webbook
tb	849.21	K	Joback Method
tc	1065.57	K	Joback Method
tf	539.39	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.53	J/molxK	849.21	Joback Method
cpg	769.72	J/molxK	885.27	Joback Method
cpg	781.86	J/molxK	921.33	Joback Method
cpg	792.96	J/molxK	957.39	Joback Method
cpg	803.08	J/molxK	993.45	Joback Method
cpg	812.24	J/molxK	1029.51	Joback Method
cpg	820.49	J/molxK	1065.57	Joback Method
dvisc	0.0004241	Paxs	539.39	Joback Method
dvisc	0.0002541	Paxs	591.03	Joback Method

dvisc	0.0001653	Paxs	642.66	Joback Method
dvisc	0.0001147	Paxs	694.30	Joback Method
dvisc	0.0000837	Paxs	745.94	Joback Method
dvisc	0.0000636	Paxs	797.57	Joback Method
dvisc	0.0000500	Paxs	849.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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