

Diethylmalonic acid, 2,3-dichlorophenyl dodecyl ester

Inchi:	InChI=1S/C25H38Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-19-30-23(28)25(5-2,6-3)24(29)3
InchiKey:	KKCOBXBFIRKSDE-UHFFFAOYSA-N
Formula:	C25H38Cl2O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	473.47

Physical Properties

Property code	Value	Unit	Source
gf	-236.09	kJ/mol	Joback Method
hf	-875.57	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	100.63	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.169		Crippen Method
mcvol	378.710	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	3032.00		NIST Webbook
tb	1032.25	K	Joback Method
tc	1263.93	K	Joback Method
tf	629.55	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1231.13	J/molxK	1032.25	Joback Method
cpg	1246.05	J/molxK	1070.86	Joback Method
cpg	1259.58	J/molxK	1109.48	Joback Method
cpg	1271.80	J/molxK	1148.09	Joback Method
cpg	1282.79	J/molxK	1186.70	Joback Method
cpg	1292.61	J/molxK	1225.31	Joback Method
cpg	1301.36	J/molxK	1263.93	Joback Method
dvisc	0.0001617	Paxs	629.55	Joback Method
dvisc	0.0000888	Paxs	696.67	Joback Method

dvisc	0.0000542	Paxs	763.78	Joback Method
dvisc	0.0000358	Paxs	830.90	Joback Method
dvisc	0.0000252	Paxs	898.02	Joback Method
dvisc	0.0000186	Paxs	965.13	Joback Method
dvisc	0.0000143	Paxs	1032.25	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=U370040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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