

Diethylmalonic acid, 3,5-dichlorophenyl octyl ester

Inchi:	InChI=1S/C21H30Cl2O4/c1-4-7-8-9-10-11-12-26-19(24)21(5-2,6-3)20(25)27-18-14-16(22)
InchiKey:	HVBSJPSTLYBERT-UHFFFAOYSA-N
Formula:	C21H30Cl2O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	417.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.77	kJ/mol	Joback Method
hf	-793.01	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	91.73	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.609		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinsol	2539.00		NIST Webbook
tb	940.73	K	Joback Method
tc	1157.76	K	Joback Method
tf	584.47	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.86	J/molxK	940.73	Joback Method
cpg	1002.86	J/molxK	976.90	Joback Method
cpg	1015.68	J/molxK	1013.07	Joback Method
cpg	1027.37	J/molxK	1049.25	Joback Method
cpg	1037.98	J/molxK	1085.42	Joback Method
cpg	1047.56	J/molxK	1121.59	Joback Method
cpg	1056.16	J/molxK	1157.76	Joback Method
dvisc	0.0002679	Paxs	584.47	Joback Method
dvisc	0.0001533	Paxs	643.85	Joback Method

dvisc	0.0000964	Paxs	703.22	Joback Method
dvisc	0.0000651	Paxs	762.60	Joback Method
dvisc	0.0000466	Paxs	821.98	Joback Method
dvisc	0.0000349	Paxs	881.35	Joback Method
dvisc	0.0000271	Paxs	940.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370442&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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