

Diethylmalonic acid, decyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C23H33Cl3O4/c1-4-7-8-9-10-11-12-13-14-29-21(27)23(5-2,6-3)22(28)30-19-16
InchiKey:	LBEBQVNIQDAMIW-UHFFFAOYSA-N
Formula:	C23H33Cl3O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	479.87

Physical Properties

Property code	Value	Unit	Source
gf	-274.49	kJ/mol	Joback Method
hf	-861.50	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	101.22	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.043		Crippen Method
mvol	362.770	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	1028.90	K	Joback Method
tc	1259.85	K	Joback Method
tf	649.45	K	Joback Method
vc	1.399	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.37	J/molxK	1028.90	Joback Method
cpg	1143.54	J/molxK	1067.39	Joback Method
cpg	1155.40	J/molxK	1105.88	Joback Method
cpg	1166.02	J/molxK	1144.37	Joback Method
cpg	1175.46	J/molxK	1182.86	Joback Method
cpg	1183.78	J/molxK	1221.35	Joback Method
cpg	1191.06	J/molxK	1259.85	Joback Method
dvisc	0.0001486	Paxs	649.45	Joback Method

dvisc	0.0000878	Paxs	712.69	Joback Method
dvisc	0.0000566	Paxs	775.93	Joback Method
dvisc	0.0000389	Paxs	839.17	Joback Method
dvisc	0.0000282	Paxs	902.42	Joback Method
dvisc	0.0000214	Paxs	965.66	Joback Method
dvisc	0.0000167	Paxs	1028.90	Joback Method

Sources

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=U370552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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