

Diethylmalonic acid, 3,5-dichlorophenyl undecyl ester

Inchi:	InChI=1S/C24H36Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-29-22(27)24(5-2,6-3)23(28)30-2
InchiKey:	UJZZCVFZDZVUGL-UHFFFAOYSA-N
Formula:	C24H36Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	459.45

Physical Properties

Property code	Value	Unit	Source
gf	-244.51	kJ/mol	Joback Method
hf	-854.93	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.779		Crippen Method
mvol	364.620	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	1009.37	K	Joback Method
tc	1235.86	K	Joback Method
tf	618.28	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.80	J/molxK	1009.37	Joback Method
cpg	1230.52	J/molxK	1198.11	Joback Method
cpg	1220.75	J/molxK	1160.37	Joback Method
cpg	1209.87	J/molxK	1122.62	Joback Method
cpg	1197.79	J/molxK	1084.87	Joback Method
cpg	1184.46	J/molxK	1047.12	Joback Method
cpg	1239.24	J/molxK	1235.86	Joback Method
dvisc	0.0000168	Paxs	1009.37	Joback Method

dvisc	0.0000218	Paxs	944.19	Joback Method
dvisc	0.0000294	Paxs	879.01	Joback Method
dvisc	0.0000417	Paxs	813.82	Joback Method
dvisc	0.0000628	Paxs	748.64	Joback Method
dvisc	0.0001021	Paxs	683.46	Joback Method
dvisc	0.0001841	Paxs	618.28	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=U370445&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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