

Dimethylmalonic acid, 2,3,5-trichlorophenyl undecyl ester

Inchi:	InChI=1S/C22H31Cl3O4/c1-4-5-6-7-8-9-10-11-12-13-28-20(26)22(2,3)21(27)29-18-15-16
InchiKey:	YUGPHPBMDNFPSW-UHFFFAOYSA-N
Formula:	C22H31Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	465.84

Physical Properties

Property code	Value	Unit	Source
gf	-282.91	kJ/mol	Joback Method
hf	-840.86	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2924.00		NIST Webbook
rinpol	2924.00		NIST Webbook
tb	1006.02	K	Joback Method
tc	1232.99	K	Joback Method
tf	638.18	K	Joback Method
vc	1.343	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.18	J/molxK	1006.02	Joback Method
cpg	1122.99	J/molxK	1195.16	Joback Method
cpg	1114.70	J/molxK	1157.33	Joback Method
cpg	1105.33	J/molxK	1119.51	Joback Method
cpg	1094.83	J/molxK	1081.68	Joback Method
cpg	1083.13	J/molxK	1043.85	Joback Method
cpg	1130.26	J/molxK	1232.99	Joback Method
dvisc	0.0000196	Paxs	1006.02	Joback Method

dvisc	0.0000250	Paxs	944.71	Joback Method
dvisc	0.0000330	Paxs	883.41	Joback Method
dvisc	0.0000452	Paxs	822.10	Joback Method
dvisc	0.0000654	Paxs	760.79	Joback Method
dvisc	0.0001007	Paxs	699.49	Joback Method
dvisc	0.0001686	Paxs	638.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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