

Dimethylmalonic acid, 2,5-dichlorophenyl dodecyl ester

Inchi:	InChI=1S/C23H34Cl2O4/c1-4-5-6-7-8-9-10-11-12-13-16-28-21(26)23(2,3)22(27)29-20-17
InchiKey:	RHXWTILLHPZYAS-UHFFFAOYSA-N
Formula:	C23H34Cl2O4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	445.42

Physical Properties

Property code	Value	Unit	Source
gf	-252.93	kJ/mol	Joback Method
hf	-834.29	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	96.18	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.389		Crippen Method
mvol	350.530	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2818.00		NIST Webbook
rinpol	2818.00		NIST Webbook
tb	986.49	K	Joback Method
tc	1208.86	K	Joback Method
tf	607.01	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.95	J/molxK	986.49	Joback Method
cpg	1123.37	J/molxK	1023.55	Joback Method
cpg	1136.52	J/molxK	1060.61	Joback Method
cpg	1148.46	J/molxK	1097.67	Joback Method
cpg	1159.26	J/molxK	1134.74	Joback Method
cpg	1168.97	J/molxK	1171.80	Joback Method
cpg	1177.65	J/molxK	1208.86	Joback Method
dvisc	0.0002092	Paxs	607.01	Joback Method

dvisc	0.0001172	Paxs	670.26	Joback Method
dvisc	0.0000726	Paxs	733.50	Joback Method
dvisc	0.0000485	Paxs	796.75	Joback Method
dvisc	0.0000344	Paxs	860.00	Joback Method
dvisc	0.0000255	Paxs	923.24	Joback Method
dvisc	0.0000197	Paxs	986.49	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=U363689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ 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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