

Diethylmalonic acid, 2-chlorophenyl dodecyl ester

Inchi:	InChI=1S/C25H39ClO4/c1-4-7-8-9-10-11-12-13-14-17-20-29-23(27)25(5-2,6-3)24(28)30-
InchiKey:	BERCDWWEMVEOSC-UHFFFAOYSA-N
Formula:	C25H39ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	439.03

Physical Properties

Property code	Value	Unit	Source
gf	-214.53	kJ/mol	Joback Method
hf	-848.36	kJ/mol	Joback Method
hfus	56.51	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	7.516		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinsol	2865.00		NIST Webbook
tb	989.84	K	Joback Method
tc	1211.90	K	Joback Method
tf	587.11	K	Joback Method
vc	1.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.74	J/molxK	989.84	Joback Method
cpg	1223.89	J/molxK	1026.85	Joback Method
cpg	1238.68	J/molxK	1063.86	Joback Method
cpg	1252.20	J/molxK	1100.87	Joback Method
cpg	1264.51	J/molxK	1137.88	Joback Method
cpg	1275.69	J/molxK	1174.89	Joback Method
cpg	1285.80	J/molxK	1211.90	Joback Method
dvisc	0.0002339	Paxs	587.11	Joback Method
dvisc	0.0001205	Paxs	654.23	Joback Method

dvisc	0.0000703	Paxs	721.35	Joback Method
dvisc	0.0000449	Paxs	788.47	Joback Method
dvisc	0.0000308	Paxs	855.60	Joback Method
dvisc	0.0000223	Paxs	922.72	Joback Method
dvisc	0.0000169	Paxs	989.84	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=U369623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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