

Diethylmalonic acid, dodecyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C25H37Cl3O4/c1-4-7-8-9-10-11-12-13-14-15-16-31-23(29)25(5-2,6-3)24(30)32
InchiKey:	GLPWYPTUEFPJOX-UHFFFAOYSA-N
Formula:	C25H37Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	507.92

Physical Properties

Property code	Value	Unit	Source
gf	-257.65	kJ/mol	Joback Method
hf	-902.78	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	105.68	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.823		Crippen Method
mcvol	390.950	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1074.66	K	Joback Method
tc	1316.85	K	Joback Method
tf	671.99	K	Joback Method
vc	1.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.13	J/molxK	1074.66	Joback Method
cpg	1306.83	J/molxK	1276.49	Joback Method
cpg	1298.45	J/molxK	1236.12	Joback Method
cpg	1288.87	J/molxK	1195.76	Joback Method
cpg	1278.01	J/molxK	1155.39	Joback Method
cpg	1265.79	J/molxK	1115.03	Joback Method
cpg	1314.10	J/molxK	1316.85	Joback Method
dvisc	0.0000121	Paxs	1074.66	Joback Method

dvisc	0.0000155	Paxs	1007.55	Joback Method
dvisc	0.0000206	Paxs	940.44	Joback Method
dvisc	0.0000287	Paxs	873.32	Joback Method
dvisc	0.0000422	Paxs	806.21	Joback Method
dvisc	0.0000664	Paxs	739.10	Joback Method
dvisc	0.0001146	Paxs	671.99	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=U370156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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