

Diethylmalonic acid, 2,3-dichlorophenyl pentadecyl ester

Inchi:	InChI=1S/C28H44Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-33-26(31)28(5-2,6-3
InchiKey:	ZTCIZKCRXJYSSP-UHFFFAOYSA-N
Formula:	C28H44Cl2O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	515.55

Physical Properties

Property code	Value	Unit	Source
gf	-210.83	kJ/mol	Joback Method
hf	-937.49	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	107.31	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.340		Crippen Method
mcvol	420.980	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook
tb	1100.89	K	Joback Method
tc	1355.25	K	Joback Method
tf	663.36	K	Joback Method
vc	1.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.56	J/molxK	1100.89	Joback Method
cpg	1433.49	J/molxK	1143.28	Joback Method
cpg	1447.78	J/molxK	1185.68	Joback Method
cpg	1460.54	J/molxK	1228.07	Joback Method
cpg	1471.88	J/molxK	1270.46	Joback Method
cpg	1481.94	J/molxK	1312.85	Joback Method
cpg	1490.83	J/molxK	1355.25	Joback Method
dvisc	0.0001080	Paxs	663.36	Joback Method

dvisc	0.0000577	Paxs	736.28	Joback Method
dvisc	0.0000345	Paxs	809.20	Joback Method
dvisc	0.0000225	Paxs	882.12	Joback Method
dvisc	0.0000156	Paxs	955.05	Joback Method
dvisc	0.0000115	Paxs	1027.97	Joback Method
dvisc	0.0000087	Paxs	1100.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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