

Pimelic acid, 2,6-dichlorophenyl dodecyl ester

Inchi: InChI=1S/C25H38Cl2O4/c1-2-3-4-5-6-7-8-9-10-14-20-30-23(28)18-12-11-13-19-24(29)3
InchiKey: LNUMSMRZCTUBRS-UHFFFAOYSA-N
Formula: C25H38Cl2O4
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 473.47

Physical Properties

Property code	Value	Unit	Source
gf	-238.93	kJ/mol	Joback Method
hf	-866.82	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	101.93	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.313		Crippen Method
mvol	378.710	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	3168.00		NIST Webbook
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tb	1035.48	K	Joback Method
tc	1269.32	K	Joback Method
tf	627.13	K	Joback Method
vc	1.474	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.98	J/molxK	1035.48	Joback Method
cpg	1289.61	J/molxK	1230.35	Joback Method
cpg	1280.85	J/molxK	1191.37	Joback Method
cpg	1270.66	J/molxK	1152.40	Joback Method
cpg	1258.99	J/molxK	1113.43	Joback Method
cpg	1245.78	J/molxK	1074.45	Joback Method
cpg	1297.00	J/molxK	1269.32	Joback Method
dvisc	0.0000191	Paxs	1035.48	Joback Method

dvisc	0.0000245	Paxs	967.42	Joback Method
dvisc	0.0000327	Paxs	899.36	Joback Method
dvisc	0.0000456	Paxs	831.31	Joback Method
dvisc	0.0000677	Paxs	763.25	Joback Method
dvisc	0.0001085	Paxs	695.19	Joback Method
dvisc	0.0001925	Paxs	627.13	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=U416665&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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