

Pimelic acid, 2,6-dichlorophenyl pentyl ester

Inchi:	InChI=1S/C18H24Cl2O4/c1-2-3-7-13-23-16(21)11-5-4-6-12-17(22)24-18-14(19)9-8-10-15
InchiKey:	UKUUXHFMVOMRBY-UHFFFAOYSA-N
Formula:	C18H24Cl2O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc1Cl
Mol. weight [g/mol]:	375.29

Physical Properties

Property code	Value	Unit	Source
gf	-297.87	kJ/mol	Joback Method
hf	-722.34	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.583		Crippen Method
mvol	280.080	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2670.00		NIST Webbook
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tb	875.32	K	Joback Method
tc	1084.97	K	Joback Method
tf	548.24	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.47	J/molxK	875.32	Joback Method
cpg	868.21	J/molxK	1050.03	Joback Method
cpg	859.16	J/molxK	1015.09	Joback Method
cpg	849.09	J/molxK	980.15	Joback Method
cpg	837.96	J/molxK	945.20	Joback Method
cpg	825.76	J/molxK	910.26	Joback Method
cpg	876.23	J/molxK	1084.97	Joback Method
dvisc	0.0000549	Paxs	875.32	Joback Method

dvisc	0.0000691	Paxs	820.81	Joback Method
dvisc	0.0000897	Paxs	766.29	Joback Method
dvisc	0.0001212	Paxs	711.78	Joback Method
dvisc	0.0001723	Paxs	657.27	Joback Method
dvisc	0.0002609	Paxs	602.75	Joback Method
dvisc	0.0004290	Paxs	548.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416658&Units=SI

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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