

Pimelic acid, 2,6-dichlorophenyl 4-methyl-2-pentyl ester

Inchi:	InChI=1S/C19H26Cl2O4/c1-13(2)12-14(3)24-17(22)10-5-4-6-11-18(23)25-19-15(20)8-7-9
InchiKey:	TYILOVREPNXZOZ-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CC(C)CC(C)OC(=O)CCCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	389.31

Physical Properties

Property code	Value	Unit	Source
gf	-294.33	kJ/mol	Joback Method
hf	-753.54	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	87.79	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.827		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	897.32	K	Joback Method
tc	1111.08	K	Joback Method
tf	529.51	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.48	J/molxK	897.32	Joback Method
cpg	885.13	J/molxK	932.95	Joback Method
cpg	897.59	J/molxK	968.57	Joback Method
cpg	908.88	J/molxK	1004.20	Joback Method
cpg	919.01	J/molxK	1039.83	Joback Method
cpg	928.01	J/molxK	1075.45	Joback Method
cpg	935.90	J/molxK	1111.08	Joback Method
dvisc	0.0004670	Paxs	529.51	Joback Method

dvisc	0.0002502	Paxs	590.81	Joback Method
dvisc	0.0001507	Paxs	652.11	Joback Method
dvisc	0.0000991	Paxs	713.41	Joback Method
dvisc	0.0000696	Paxs	774.72	Joback Method
dvisc	0.0000515	Paxs	836.02	Joback Method
dvisc	0.0000397	Paxs	897.32	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=U416657&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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