

Pimelic acid, di(2,6-dichlorophenyl) ester

Inchi:	InChI=1S/C19H16Cl4O4/c20-12-6-4-7-13(21)18(12)26-16(24)10-2-1-3-11-17(25)27-19-1
InchiKey:	GIVSDPNYTBNQRY-UHFFFAOYSA-N
Formula:	C19H16Cl4O4
SMILES:	O=C(CCCCCC(=O)Oc1c(Cl)cccc1Cl)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	450.14

Physical Properties

Property code	Value	Unit	Source
gf	-220.16	kJ/mol	Joback Method
hf	-560.87	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	100.94	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.762		Crippen Method
mvol	294.890	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	1009.70	K	Joback Method
tc	1251.92	K	Joback Method
tf	670.81	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.65	J/molxK	1009.70	Joback Method
cpg	829.65	J/molxK	1211.55	Joback Method
cpg	826.28	J/molxK	1171.18	Joback Method
cpg	821.73	J/molxK	1130.81	Joback Method
cpg	815.96	J/molxK	1090.44	Joback Method
cpg	808.94	J/molxK	1050.07	Joback Method
cpg	831.86	J/molxK	1251.92	Joback Method
dvisc	0.0000370	Paxs	1009.70	Joback Method

dvisc	0.0000451	Paxs	953.22	Joback Method
dvisc	0.0000564	Paxs	896.74	Joback Method
dvisc	0.0000727	Paxs	840.26	Joback Method
dvisc	0.0000972	Paxs	783.77	Joback Method
dvisc	0.0001359	Paxs	727.29	Joback Method
dvisc	0.0002010	Paxs	670.81	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=U416666&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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