

Pimelic acid, 2,6-dichlorophenyl propyl ester

Inchi:	InChI=1S/C16H20Cl2O4/c1-2-11-21-14(19)9-4-3-5-10-15(20)22-16-12(17)7-6-8-13(16)18
InchiKey:	VQVXPPSULUQABR-UHFFFAOYSA-N
Formula:	C16H20Cl2O4
SMILES:	CCCOC(=O)CCCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	347.23

Physical Properties

Property code	Value	Unit	Source
gf	-314.71	kJ/mol	Joback Method
hf	-681.06	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.803		Crippen Method
mvol	251.900	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2428.00		NIST Webbook
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tb	829.56	K	Joback Method
tc	1039.86	K	Joback Method
tf	525.70	K	Joback Method
vc	0.970	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.88	J/molxK	829.56	Joback Method
cpg	711.67	J/molxK	864.61	Joback Method
cpg	723.45	J/molxK	899.66	Joback Method
cpg	734.25	J/molxK	934.71	Joback Method
cpg	744.06	J/molxK	969.76	Joback Method
cpg	752.91	J/molxK	1004.81	Joback Method
cpg	760.81	J/molxK	1039.86	Joback Method
dvisc	0.0005229	Paxs	525.70	Joback Method

dvisc	0.0003260	Paxs	576.34	Joback Method
dvisc	0.0002193	Paxs	626.99	Joback Method
dvisc	0.0001566	Paxs	677.63	Joback Method
dvisc	0.0001171	Paxs	728.27	Joback Method
dvisc	0.0000910	Paxs	778.92	Joback Method
dvisc	0.0000729	Paxs	829.56	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=U416654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	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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