

Pimelic acid, 3,4-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C15H18Cl2O4/c1-2-20-14(18)6-4-3-5-7-15(19)21-11-8-9-12(16)13(17)10-11/h
InchiKey:	GKUZYSJDOFIAG-UHFFFAOYSA-N
Formula:	C15H18Cl2O4
SMILES:	CCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	333.21

Physical Properties

Property code	Value	Unit	Source
gf	-323.13	kJ/mol	Joback Method
hf	-660.42	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.412		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	806.68	K	Joback Method
tc	1018.29	K	Joback Method
tf	514.43	K	Joback Method
vc	0.913	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.41	J/molxK	806.68	Joback Method
cpg	696.31	J/molxK	983.02	Joback Method
cpg	687.62	J/molxK	947.76	Joback Method
cpg	678.00	J/molxK	912.49	Joback Method
cpg	667.42	J/molxK	877.22	Joback Method
cpg	655.90	J/molxK	841.95	Joback Method
cpg	704.08	J/molxK	1018.29	Joback Method
dvisc	0.0000837	Paxs	806.68	Joback Method

dvisc	0.0001041	Paxs	757.97	Joback Method
dvisc	0.0001333	Paxs	709.26	Joback Method
dvisc	0.0001771	Paxs	660.56	Joback Method
dvisc	0.0002462	Paxs	611.85	Joback Method
dvisc	0.0003623	Paxs	563.14	Joback Method
dvisc	0.0005736	Paxs	514.43	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=U416727&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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