Pimelic acid, 2,6-dichlorophenyl ethyl ester

Inchi: InChI=1S/C15H18Cl2O4/c1-2-20-13(18)9-4-3-5-10-14(19)21-15-11(16)7-6-8-12(15)17/h6
InchiKey: CYAYMAUXVFOUDF-UHFFFAOYSA-N
Formula: C15H18Cl2O4
SMILES: CCOC(=O)CCCCCC(=O)Oc1c(Cl)cccc1Cl
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	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	806.68	K	Joback Method
tc	1018.29	K	Joback Method
tf	514.43	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001041	Pa×s	757.97	Joback Method
dvisc	0.0001333	Pa×s	709.26	Joback Method
dvisc	0.0001771	Pa×s	660.56	Joback Method
dvisc	0.0002462	Pa×s	611.85	Joback Method
dvisc	0.0003623	Pa×s	563.14	Joback Method
dvisc	0.0005736	Pa×s	514.43	Joback Method

Sources

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=U416653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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