Pimelic acid, 2-chlorophenyl ethyl ester

Inchi: InChI=1S/C15H19ClO4/c1-2-19-14(17)10-4-3-5-11-15(18)20-13-9-7-6-8-12(13)16/h6-9H
InchiKey: ZXZDABJKTYHALA-UHFFFAOYSA-N
Formula: C15H19ClO4
SMILES: CCOC(=O)CCCCCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-301.57	kJ/mol	Joback Method
hf	-633.21	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.759		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	764.27	K	Joback Method
tc	971.48	K	Joback Method
tf	471.99	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.06	J/mol×K	764.27	Joback Method
cpg	633.75	J/mol×K	798.81	Joback Method
cpg	646.48	J/mol×K	833.34	Joback Method
cpg	658.28	J/mol×K	867.88	Joback Method
cpg	669.14	J/mol×K	902.41	Joback Method
cpg	679.09	J/mol×K	936.95	Joback Method
cpg	688.14	J/mol×K	971.48	Joback Method
dvisc	0.0007853	Pa×s	471.99	Joback Method

dvisc	0.0004679	Pa×s	520.70	Joback Method
dvisc	0.0003046	Pa×s	569.42	Joback Method
dvisc	0.0002121	Pa×s	618.13	Joback Method
dvisc	0.0001558	Pa×s	666.84	Joback Method
dvisc	0.0001193	Pa×s	715.56	Joback Method
dvisc	0.0000945	Pa×s	764.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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