

Pimelic acid, 4-chlorophenyl ethyl ester

Inchi:	InChI=1S/C15H19ClO4/c1-2-19-14(17)6-4-3-5-7-15(18)20-13-10-8-12(16)9-11-13/h8-11H
InchiKey:	ZHANIAQPYFULIM-UHFFFAOYSA-N
Formula:	C15H19ClO4
SMILES:	CCOC(=O)CCCCC(=O)Oc1ccc(Cl)cc1
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
mvol	225.570	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	764.27	K	Joback Method
tc	971.48	K	Joback Method
tf	471.99	K	Joback Method
vc	0.865	m ³ /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	Paxs	471.99	Joback Method

dvisc	0.0004679	Paxs	520.70	Joback Method
dvisc	0.0003046	Paxs	569.42	Joback Method
dvisc	0.0002121	Paxs	618.13	Joback Method
dvisc	0.0001558	Paxs	666.84	Joback Method
dvisc	0.0001193	Paxs	715.56	Joback Method
dvisc	0.0000945	Paxs	764.27	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=U393826&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

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