

Pimelic acid, 4-chloro-3-methylphenyl propyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-3-11-21-16(19)7-5-4-6-8-17(20)22-14-9-10-15(18)13(2)12-14
InchiKey:	KQWQNKQVFZPCGB-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-294.36	kJ/mol	Joback Method
hf	-685.96	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.458		Crippen Method
mvol	253.750	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2426.00		NIST Webbook
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tb	815.01	K	Joback Method
tc	1020.37	K	Joback Method
tf	507.05	K	Joback Method
vc	0.977	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.36	J/molxK	815.01	Joback Method
cpg	791.23	J/molxK	986.14	Joback Method
cpg	781.06	J/molxK	951.91	Joback Method
cpg	769.90	J/molxK	917.69	Joback Method
cpg	757.73	J/molxK	883.46	Joback Method
cpg	744.56	J/molxK	849.24	Joback Method
cpg	800.43	J/molxK	1020.37	Joback Method
dvisc	0.0000730	Paxs	815.01	Joback Method

dvisc	0.0000915	Paxs	763.68	Joback Method
dvisc	0.0001187	Paxs	712.36	Joback Method
dvisc	0.0001601	Paxs	661.03	Joback Method
dvisc	0.0002273	Paxs	609.70	Joback Method
dvisc	0.0003441	Paxs	558.38	Joback Method
dvisc	0.0005664	Paxs	507.05	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=U416681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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