

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

Inchi:	InChI=1S/C16H21ClO4/c1-3-20-15(18)7-5-4-6-8-16(19)21-13-9-10-14(17)12(2)11-13/h9-
InchiKey:	SSUAIAWNTIKCJV-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-302.78	kJ/mol	Joback Method
hf	-665.32	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.067		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	792.13	K	Joback Method
tc	998.52	K	Joback Method
tf	495.78	K	Joback Method
vc	0.920	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.17	J/molxK	792.13	Joback Method
cpg	688.09	J/molxK	826.53	Joback Method
cpg	701.02	J/molxK	860.93	Joback Method
cpg	712.98	J/molxK	895.32	Joback Method
cpg	723.98	J/molxK	929.72	Joback Method
cpg	734.02	J/molxK	964.12	Joback Method
cpg	743.12	J/molxK	998.52	Joback Method
dvisc	0.0006188	Paxs	495.78	Joback Method

dvisc	0.0003809	Paxs	545.17	Joback Method
dvisc	0.0002541	Paxs	594.56	Joback Method
dvisc	0.0001804	Paxs	643.96	Joback Method
dvisc	0.0001345	Paxs	693.35	Joback Method
dvisc	0.0001042	Paxs	742.74	Joback Method
dvisc	0.0000834	Paxs	792.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416680&Units=SI
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

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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