

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

Inchi:	InChI=1S/C19H27ClO4/c1-3-4-8-13-23-18(21)9-6-5-7-10-19(22)24-16-11-12-17(20)15(2)
InchiKey:	LEBJHBRWKTUVCY-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-277.52	kJ/mol	Joback Method
hf	-727.24	kJ/mol	Joback Method
hfus	48.00	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.238		Crippen Method
mvol	281.930	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rmpol	2663.00		NIST Webbook
tb	860.77	K	Joback Method
tc	1066.00	K	Joback Method
tf	529.59	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.41	J/molxK	860.77	Joback Method
cpg	860.08	J/molxK	894.98	Joback Method
cpg	873.64	J/molxK	929.18	Joback Method
cpg	886.11	J/molxK	963.39	Joback Method
cpg	897.50	J/molxK	997.59	Joback Method
cpg	907.83	J/molxK	1031.80	Joback Method
cpg	917.12	J/molxK	1066.00	Joback Method
dvisc	0.0004680	Paxs	529.59	Joback Method
dvisc	0.0002772	Paxs	584.79	Joback Method

dvisc	0.0001797	Paxs	639.98	Joback Method
dvisc	0.0001248	Paxs	695.18	Joback Method
dvisc	0.0000915	Paxs	750.38	Joback Method
dvisc	0.0000699	Paxs	805.57	Joback Method
dvisc	0.0000554	Paxs	860.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416685&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mvol:	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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