

Pimelic acid, 3-chlorophenyl undecyl ester

Inchi:	InChI=1S/C24H37ClO4/c1-2-3-4-5-6-7-8-9-13-19-28-23(26)17-11-10-12-18-24(27)29-22
InchiKey:	FTDQRJJMQNSUEZ-UHFFFAOYSA-N
Formula:	C24H37ClO4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	425.00

Physical Properties

Property code	Value	Unit	Source
gf	-225.79	kJ/mol	Joback Method
hf	-818.97	kJ/mol	Joback Method
hfus	61.34	kJ/mol	Joback Method
hvap	94.65	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.270		Crippen Method
mvol	352.380	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	970.19	K	Joback Method
tc	1187.80	K	Joback Method
tf	573.42	K	Joback Method
vc	1.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.11	J/molxK	970.19	Joback Method
cpg	1161.98	J/molxK	1006.46	Joback Method
cpg	1176.44	J/molxK	1042.73	Joback Method
cpg	1189.54	J/molxK	1079.00	Joback Method
cpg	1201.32	J/molxK	1115.26	Joback Method
cpg	1211.83	J/molxK	1151.53	Joback Method
cpg	1221.10	J/molxK	1187.80	Joback Method
dvisc	0.0003068	Paxs	573.42	Joback Method

dvisc	0.0001644	Paxs	639.55	Joback Method
dvisc	0.0000990	Paxs	705.68	Joback Method
dvisc	0.0000650	Paxs	771.81	Joback Method
dvisc	0.0000457	Paxs	837.93	Joback Method
dvisc	0.0000338	Paxs	904.06	Joback Method
dvisc	0.0000260	Paxs	970.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416677&Units=SI

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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