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

Inchi: InChI=1S/C23H35ClO4/c1-3-4-5-6-7-8-12-17-27-22(25)13-10-9-11-14-23(26)28-20-15-16

InchiKey: MWYRGKUICCSWOX-UHFFFAOYSA-N

Formula: C23H35ClO4

SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 410.98

Physical Properties

Property code	Value	Unit	Source
gf	-243.84	kJ/mol	Joback Method
hf	-809.80	kJ/mol	Joback Method
hfus	58.36	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.798		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	952.29	K	Joback Method
tc	1166.50	K	Joback Method
tf	574.67	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.19	J/mol×K	952.29	Joback Method
cpg	1148.57	J/mol×K	1130.80	Joback Method
cpg	1138.27	J/mol×K	1095.10	Joback Method
cpg	1126.72	J/mol×K	1059.39	Joback Method
cpg	1113.87	J/mol×K	1023.69	Joback Method
cpg	1099.71	J/mol×K	987.99	Joback Method
cpg	1157.64	J/mol×K	1166.50	Joback Method
dvisc	0.0000309	Pa×s	952.29	Joback Method

dvisc	0.0000396	Pa×s	889.35	Joback Method
dvisc	0.0000526	Pa×s	826.42	Joback Method
dvisc	0.0000732	Pa×s	763.48	Joback Method
dvisc	0.0001081	Pa×s	700.54	Joback Method
dvisc	0.0001724	Pa×s	637.61	Joback Method
dvisc	0.0003047	Pa×s	574.67	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=U416689&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