Pimelic acid, 3-chlorophenyl propyl ester

Inchi: InChI=1S/C16H21ClO4/c1-2-11-20-15(18)9-4-3-5-10-16(19)21-14-8-6-7-13(17)12-14/h6-
InchiKey: CJMHDVQHERZWPK-UHFFFAOYSA-N
Formula: C16H21ClO4
SMILES: CCCOC(=O)CCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-293.15	kJ/mol	Joback Method
hf	-653.85	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	76.85	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.149		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	787.15	K	Joback Method
tc	992.74	K	Joback Method
tf	483.26	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.20	J/mol×K	787.15	Joback Method
cpg	689.21	J/mol×K	821.42	Joback Method
cpg	702.22	J/mol×K	855.68	Joback Method
cpg	714.27	J/mol×K	889.95	Joback Method
cpg	725.35	J/mol×K	924.21	Joback Method
cpg	735.49	J/mol×K	958.48	Joback Method
cpg	744.69	J/mol×K	992.74	Joback Method
dvisc	0.0007196	Pa×s	483.26	Joback Method

dvisc	0.0004230	Pa×s	533.91	Joback Method
dvisc	0.0002726	Pa×s	584.56	Joback Method
dvisc	0.0001884	Pa×s	635.21	Joback Method
dvisc	0.0001376	Pa×s	685.85	Joback Method
dvisc	0.0001049	Pa×s	736.50	Joback Method
dvisc	0.0000828	Pa×s	787.15	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=U416668&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