Pimelic acid, 4-chlorobenzyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C20H29ClO4/c1-15(2)13-16(3)25-20(23)8-6-4-5-7-19(22)24-14-17-9-11-18(21)

InchiKey: BUUUGGKMBJHBMH-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-264.35	kJ/mol	Joback Method
hf	-746.97	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.311		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	877.79	K	Joback Method
tc	1086.31	K	Joback Method
tf	498.34	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.98	J/mol×K	877.79	Joback Method
cpg	921.13	J/mol×K	912.54	Joback Method
cpg	935.07	J/mol×K	947.30	Joback Method
cpg	947.83	J/mol×K	982.05	Joback Method
cpg	959.44	J/mol×K	1016.81	Joback Method
cpg	969.91	J/mol×K	1051.56	Joback Method
cpg	979.28	J/mol×K	1086.31	Joback Method
dvisc	0.0006126	Pa×s	498.34	Joback Method

dvisc	0.0003000	Pa×s	561.58	Joback Method
dvisc	0.0001698	Pa×s	624.82	Joback Method
dvisc	0.0001067	Pa×s	688.07	Joback Method
dvisc	0.0000725	Pa×s	751.31	Joback Method
dvisc	0.0000523	Pa×s	814.55	Joback Method
dvisc	0.0000395	Pa×s	877.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406795&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