

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)CCCCC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003000	Paxs	561.58	Joback Method
dvisc	0.0001698	Paxs	624.82	Joback Method
dvisc	0.0001067	Paxs	688.07	Joback Method
dvisc	0.0000725	Paxs	751.31	Joback Method
dvisc	0.0000523	Paxs	814.55	Joback Method
dvisc	0.0000395	Paxs	877.79	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=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

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