

Pimelic acid, 5-chloro-2-nitrobenzyl octyl ester

Inchi:	InChI=1S/C22H32ClNO6/c1-2-3-4-5-6-10-15-29-21(25)11-8-7-9-12-22(26)30-17-18-16-1
InchiKey:	KQWHEKXVCM TIPZ-UHFFFAOYSA-N
Formula:	C22H32ClNO6
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	441.95

Physical Properties

Property code	Value	Unit	Source
gf	-216.71	kJ/mol	Joback Method
hf	-799.92	kJ/mol	Joback Method
hfus	67.13	kJ/mol	Joback Method
hvap	107.45	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.146		Crippen Method
mvol	341.620	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	3179.00		NIST Webbook
rinpol	3179.00		NIST Webbook
tb	1081.25	K	Joback Method
tc	1323.87	K	Joback Method
tf	707.01	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.96	J/molxK	1081.25	Joback Method
cpg	1138.28	J/molxK	1121.69	Joback Method
cpg	1148.02	J/molxK	1162.12	Joback Method
cpg	1156.25	J/molxK	1202.56	Joback Method
cpg	1163.00	J/molxK	1243.00	Joback Method
cpg	1168.33	J/molxK	1283.44	Joback Method
cpg	1172.30	J/molxK	1323.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U406704&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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