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

Inchi: InChI=1S/C21H30ClNO6/c1-2-3-4-5-9-14-28-20(24)10-7-6-8-11-21(25)29-16-17-15-18(2

InchiKey: HAHKYMRTOIPVBE-UHFFFAOYSA-N

Formula: C21H30ClNO6

SMILES: CCCCCCCOC(=O)CCCCCC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 427.92

Physical Properties

Property code	Value	Unit	Source
gf	-225.13	kJ/mol	Joback Method
hf	-779.28	kJ/mol	Joback Method
hfus	64.54	kJ/mol	Joback Method
hvap	105.23	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.755		Crippen Method
mcvol	327.530	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	3081.00		NIST Webbook
rinpol	3081.00		NIST Webbook
tb	1058.37	K	Joback Method
tc	1295.91	K	Joback Method
tf	695.74	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.03	J/mol×K	1058.37	Joback Method
cpg	1078.26	J/mol×K	1097.96	Joback Method
cpg	1088.01	J/mol×K	1137.55	Joback Method
cpg	1096.30	J/mol×K	1177.14	Joback Method
cpg	1103.20	J/mol×K	1216.73	Joback Method
cpg	1108.74	J/mol×K	1256.32	Joback Method
cpg	1112.96	J/mol×K	1295.91	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=U406703&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
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