Pimelic acid, 5-chloro-2-nitrobenzyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C20H28ClNO6/c1-14(2)11-15(3)28-20(24)8-6-4-5-7-19(23)27-13-16-12-17(21)9-10-18(16)22(25)26/h9-10,12,14-15H,4-8,11,13H2,1-3H3

InchiKey: VGYKYVHGHNLMEZ-UHFFFAOYSA-N

Formula: C20H28ClNO6

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 413.89

Physical Properties

Property code	Value	Unit	Source
gf	-238.43	kJ/mol	Joback Method
hf	-769.20	kJ/mol	Joback Method
hfus	54.90	kJ/mol	Joback Method
hvap	102.23	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.220		Crippen Method
mcvol	313.440	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2835.00		NIST Webbook
rinpol	2835.00		NIST Webbook
tb	1034.61	K	Joback Method
tc	1269.63	K	Joback Method
tf	654.47	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.16	J/mol×K	1034.61	Joback Method
cpg	1019.21	J/mol×K	1073.78	Joback Method
cpg	1028.79	J/mol×K	1112.95	Joback Method
cpg	1036.95	J/mol×K	1152.12	Joback Method
cpg	1043.72	J/mol×K	1191.29	Joback Method
cpg	1049.13	J/mol×K	1230.46	Joback Method
cpg	1053.24	J/mol×K	1269.63	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=U406700&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