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

Inchi: InChI=1S/C19H26ClNO6/c1-2-3-7-12-26-18(22)8-5-4-6-9-19(23)27-14-15-13-16(20)10-1

InchiKey: KMSTWFPPFXCRMZ-UHFFFAOYSA-N

Formula: C19H26ClNO6

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

Mol. weight [g/mol]: 399.87

Physical Properties

Property code	Value	Unit	Source
gf	-241.97	kJ/mol	Joback Method
hf	-738.00	kJ/mol	Joback Method
hfus	59.36	kJ/mol	Joback Method
hvap	100.78	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.975		Crippen Method
mcvol	299.350	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2883.00		NIST Webbook
rinpol	2883.00		NIST Webbook
tb	1012.61	K	Joback Method
tc	1243.24	K	Joback Method
tf	673.20	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.42	J/mol×K	1012.61	Joback Method
cpg	959.47	J/mol×K	1051.05	Joback Method
cpg	969.17	J/mol×K	1089.49	Joback Method
cpg	977.55	J/mol×K	1127.93	Joback Method
cpg	984.64	J/mol×K	1166.36	Joback Method
cpg	990.48	J/mol×K	1204.80	Joback Method
cpg	995.09	J/mol×K	1243.24	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=U406701&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