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

Inchi: InChI=1S/C17H22ClNO6/c1-2-10-24-16(20)6-4-3-5-7-17(21)25-12-13-11-14(18)8-9-15(1

InchiKey: XBPUOSMTTMTGIH-UHFFFAOYSA-N

Formula: C17H22ClNO6

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

Mol. weight [g/mol]: 371.81

Physical Properties

Property code	Value	Unit	Source
gf	-258.81	kJ/mol	Joback Method
hf	-696.72	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	96.32	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.195		Crippen Method
mcvol	271.170	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
tb	966.85	K	Joback Method
tc	1194.49	K	Joback Method
tf	650.66	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.77	J/mol×K	966.85	Joback Method
cpg	842.61	J/mol×K	1004.79	Joback Method
cpg	852.20	J/mol×K	1042.73	Joback Method
cpg	860.58	J/mol×K	1080.67	Joback Method
cpg	867.75	J/mol×K	1118.61	Joback Method
cpg	873.74	J/mol×K	1156.55	Joback Method
cpg	878.57	J/mol×K	1194.49	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=U406697&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