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

Inchi: InChI=1S/C16H20ClNO6/c1-2-23-15(19)6-4-3-5-7-16(20)24-11-12-10-13(17)8-9-14(12)1
InchiKey: NVQQMSDALOVDEQ-UHFFFAOYSA-N
Formula: C16H20ClNO6
SMILES: CCOC(=O)CCCCCC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 357.79

Physical Properties

Property code	Value	Unit	Source
gf	-267.23	kJ/mol	Joback Method
hf	-676.08	kJ/mol	Joback Method
hfus	51.59	kJ/mol	Joback Method
hvap	94.10	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.805		Crippen Method
mcvol	257.080	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	943.97	K	Joback Method
tc	1171.44	K	Joback Method
tf	639.39	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.31	J/mol×K	943.97	Joback Method
cpg	785.02	J/mol×K	981.88	Joback Method
cpg	794.53	J/mol×K	1019.79	Joback Method
cpg	802.86	J/mol×K	1057.70	Joback Method
cpg	810.02	J/mol×K	1095.61	Joback Method
cpg	816.03	J/mol×K	1133.52	Joback Method
cpg	820.92	J/mol×K	1171.44	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=U406696&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