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

Inchi: InChI=1S/C18H24ClNO6/c1-13(2)11-25-17(21)6-4-3-5-7-18(22)26-12-14-10-15(19)8-9-1

InchiKey: VRQOCLNTNQMZNI-UHFFFAOYSA-N

Formula: C18H24ClNO6

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

Mol. weight [g/mol]: 385.84

Physical Properties

Property code	Value	Unit	Source
gf	-252.83	kJ/mol	Joback Method
hf	-722.64	kJ/mol	Joback Method
hfus	53.25	kJ/mol	Joback Method
hvap	98.16	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.441		Crippen Method
mcvol	285.260	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	989.29	K	Joback Method
tc	1219.41	K	Joback Method
tf	646.93	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.24	J/mol×K	989.29	Joback Method
cpg	901.20	J/mol×K	1027.64	Joback Method
cpg	910.83	J/mol×K	1066.00	Joback Method
cpg	919.16	J/mol×K	1104.35	Joback Method
cpg	926.22	J/mol×K	1142.70	Joback Method
cpg	932.03	J/mol×K	1181.06	Joback Method
cpg	936.62	J/mol×K	1219.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406698&Units=SI
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

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