8-Chlorooctyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C15H19ClN2O6/c16-7-5-3-1-2-4-6-8-24-15(19)12-9-13(17(20)21)11-14(10-12)
InchiKey: XYJFAXKBTUZNEO-UHFFFAOYSA-N
Formula: C15H19ClN2O6
SMILES: O=C(OCCCCCCCCCCl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 358.77

Physical Properties

Property code	Value	Unit	Source
gf	-6.18	kJ/mol	Joback Method
hf	-421.40	kJ/mol	Joback Method
hfus	57.57	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.239		Crippen Method
mcvol	252.970	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	996.64	K	Joback Method
tc	1238.89	K	Joback Method
tf	699.57	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.98	J/mol×K	996.64	Joback Method
cpg	785.79	J/mol×K	1037.01	Joback Method
cpg	794.50	J/mol×K	1077.39	Joback Method
cpg	802.16	J/mol×K	1117.76	Joback Method
cpg	808.81	J/mol×K	1158.14	Joback Method
cpg	814.50	J/mol×K	1198.51	Joback Method
cpg	819.29	J/mol×K	1238.89	Joback Method

Sources

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=U373866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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