2-(2-Ethoxyethoxy)ethyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C13H16N2O8/c1-2-21-3-4-22-5-6-23-13(16)10-7-11(14(17)18)9-12(8-10)15(19
InchiKey: IBROIYRFSMWSLH-UHFFFAOYSA-N
Formula: C13H16N2O8
SMILES: CCOCCOCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 328.27

Physical Properties

Property code	Value	Unit	Source
gf	-221.09	kJ/mol	Joback Method
hf	-628.82	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	95.29	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	1.713		Crippen Method
mcvol	224.290	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	958.29	K	Joback Method
tc	1198.24	K	Joback Method
tf	691.57	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.01	J/mol×K	958.29	Joback Method
cpg	702.03	J/mol×K	998.28	Joback Method
cpg	709.67	J/mol×K	1038.27	Joback Method
cpg	715.94	J/mol×K	1078.26	Joback Method
cpg	720.82	J/mol×K	1118.25	Joback Method
cpg	724.31	J/mol×K	1158.25	Joback Method
cpg	726.40	J/mol×K	1198.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378309&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