2-Ethoxyethyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C11H12N2O7/c1-2-19-3-4-20-11(14)8-5-9(12(15)16)7-10(6-8)13(17)18/h5-7H,
InchiKey: SCXGAVJIYIXEAJ-UHFFFAOYSA-N
Formula: C11H12N2O7
SMILES: CCOCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 284.22

Physical Properties

Property code	Value	Unit	Source
gf	-132.93	kJ/mol	Joback Method
hf	-455.32	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	88.43	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	1.696		Crippen Method
mcvol	190.240	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	890.11	K	Joback Method
tc	1137.51	K	Joback Method
tf	646.80	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.05	J/mol×K	890.11	Joback Method
cpg	567.52	J/mol×K	931.34	Joback Method
cpg	575.82	J/mol×K	972.58	Joback Method
cpg	582.97	J/mol×K	1013.81	Joback Method
cpg	588.96	J/mol×K	1055.04	Joback Method
cpg	593.82	J/mol×K	1096.28	Joback Method
cpg	597.54	J/mol×K	1137.51	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=U378311&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