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

Inchi: InChI=1S/C12H14N2O8/c1-20-2-3-21-4-5-22-12(15)9-6-10(13(16)17)8-11(7-9)14(18)19/
InchiKey: MPRFLYOPKSBFJK-UHFFFAOYSA-N
Formula: C12H14N2O8
SMILES: COCCOCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 314.25

Physical Properties

Property code	Value	Unit	Source
gf	-229.51	kJ/mol	Joback Method
hf	-608.18	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	93.06	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	1.323		Crippen Method
mcvol	210.200	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	935.41	K	Joback Method
tc	1177.42	K	Joback Method
tf	680.30	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.14	J/mol×K	935.41	Joback Method
cpg	646.07	J/mol×K	975.75	Joback Method
cpg	653.66	J/mol×K	1016.08	Joback Method
cpg	659.92	J/mol×K	1056.42	Joback Method
cpg	664.82	J/mol×K	1096.75	Joback Method
cpg	668.36	J/mol×K	1137.09	Joback Method
cpg	670.53	J/mol×K	1177.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378310&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