2-Butoxyethyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C13H16N2O7/c1-2-3-4-21-5-6-22-13(16)10-7-11(14(17)18)9-12(8-10)15(19)20
InchiKey: GPEWXIVENNPUPI-UHFFFAOYSA-N
Formula: C13H16N2O7
SMILES: CCCCOCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 312.28

Physical Properties

Property code	Value	Unit	Source
gf	-116.09	kJ/mol	Joback Method
hf	-496.60	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	92.88	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.476		Crippen Method
mcvol	218.420	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	935.87	K	Joback Method
tc	1177.08	K	Joback Method
tf	669.34	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.70	J/mol×K	935.87	Joback Method
cpg	678.58	J/mol×K	976.07	Joback Method
cpg	687.24	J/mol×K	1016.27	Joback Method
cpg	694.69	J/mol×K	1056.47	Joback Method
cpg	700.95	J/mol×K	1096.67	Joback Method
cpg	706.02	J/mol×K	1136.88	Joback Method
cpg	709.94	J/mol×K	1177.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378312&Units=SI

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