1-Butoxypropan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C14H18N2O7/c1-3-4-5-22-9-10(2)23-14(17)11-6-12(15(18)19)8-13(7-11)16(20
InchiKey: FVUZKXJWGVSKJT-UHFFFAOYSA-N
Formula: C14H18N2O7
SMILES: CCCCOCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 326.30

Physical Properties

Property code	Value	Unit	Source
gf	-110.11	kJ/mol	Joback Method
hf	-522.52	kJ/mol	Joback Method
hfus	48.45	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	2.865		Crippen Method
mcvol	232.510	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	958.31	K	Joback Method
tc	1200.34	K	Joback Method
tf	665.61	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.63	J/mol×K	958.31	Joback Method
cpg	735.70	J/mol×K	998.65	Joback Method
cpg	744.47	J/mol×K	1038.99	Joback Method
cpg	751.96	J/mol×K	1079.33	Joback Method
cpg	758.19	J/mol×K	1119.66	Joback Method
cpg	763.18	J/mol×K	1160.00	Joback Method
cpg	766.95	J/mol×K	1200.34	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=U378313&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