

2-Bromo-1-(4-nitrophenyl)ethyl nitrate

Inchi:	InChI=1S/C8H7BrN2O5/c9-5-8(16-11(14)15)6-1-3-7(4-2-6)10(12)13/h1-4,8H,5H2
InchiKey:	APCSUXLRGPGZCG-UHFFFAOYSA-N
Formula:	C8H7BrN2O5
SMILES:	O=[N+]([O-])OC(CBr)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	291.06
CAS:	90221-54-8

Physical Properties

Property code	Value	Unit	Source
gf	97.24	kJ/mol	Joback Method
hf	-116.08	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.239		Crippen Method
mcvol	158.030	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	805.92	K	Joback Method
tc	1082.03	K	Joback Method
tf	573.11	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.57	J/molxK	805.92	Joback Method
cpg	408.55	J/molxK	851.94	Joback Method
cpg	416.55	J/molxK	897.96	Joback Method
cpg	423.62	J/molxK	943.98	Joback Method
cpg	429.82	J/molxK	989.99	Joback Method
cpg	435.22	J/molxK	1036.01	Joback Method
cpg	439.88	J/molxK	1082.03	Joback Method

Sources

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=C90221548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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