Benzene, 1-(2-bromoethyl)-4-nitro-

Other names:	«beta»-(p-Nitrophenyl)ethyl bromide
	p-Nitrophenethyl bromide
	1-(2-Bromoethyl)-4-nitrobenzene
	2-(4-Nitrophenyl)ethyl bromide
	4-(2-Bromoethyl)nitrobenzene
	1-Bromo-2-(4-nitrophenyl)ethane
	4-nitrophenethyl bromide
Inchi:	InChI=1S/C8H8BrNO2/c9-6-5-7-1-3-8(4-2-7)10(11)12/h1-4H,5-6H2
InchiKey:	NTURQZFFJDCTMZ-UHFFFAOYSA-N
Formula:	C8H8BrNO2
SMILES:	O=[N+]([O-])c1ccc(CCBr)cc1
Mol. weight [g/mol]:	230.06
CAS:	5339-26-4

Physical Properties

Property code	Value	Unit	Source
gf	169.13	kJ/mol	Joback Method
hf	32.18	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	59.37	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-3.36		Crippen Method
logp	2.532		Crippen Method
mcvol	134.740	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	632.10	K	Joback Method
tc	889.86	K	Joback Method
tf	422.27	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.03	J/mol×K	632.10	Joback Method

cpg	307.93	J/mol×K	675.06	Joback Method
cpg	317.93	J/mol×K	718.02	Joback Method
cpg	327.09	J/mol×K	760.98	Joback Method
cpg	335.48	J/mol×K	803.94	Joback Method
cpg	343.16	J/mol×K	846.90	Joback Method
cpg	350.21	J/mol×K	889.86	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=C5339264&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
ie:	Ionization energy
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