

p-Nitrophenyl bromoacetate

Other names:	4-Nitrophenyl bromoacetate Bromoacetic acid, 4-nitrophenyl ester Acetic acid, 2-bromo-, 4-nitrophenyl ester
Inchi:	InChI=1S/C8H6BrNO4/c9-5-8(11)14-7-3-1-6(2-4-7)10(12)13/h1-4H,5H2
InchiKey:	HVNXGOPARVAZNX-UHFFFAOYSA-N
Formula:	C8H6BrNO4
SMILES:	O=C(CBr)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	260.04
CAS:	19199-82-7

Physical Properties

Property code	Value	Unit	Source
gf	-64.79	kJ/mol	Joback Method
hf	-212.62	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.895		Crippen Method
mcvol	142.180	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook
tb	708.39	K	Joback Method
tc	967.12	K	Joback Method
tf	494.43	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.41	J/molxK	708.39	Joback Method
cpg	335.62	J/molxK	751.51	Joback Method
cpg	343.98	J/molxK	794.63	Joback Method
cpg	351.53	J/molxK	837.75	Joback Method

cpg	358.31	J/mol×K	880.88	Joback Method
cpg	364.35	J/mol×K	924.00	Joback Method
cpg	369.69	J/mol×K	967.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C19199827&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
mvol:	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

Latest version available from:

<https://www.cheméo.com/cid/19-647-3/p-Nitrophenyl-bromoacetate.pdf>

Generated by Cheméo on 2024-04-19 20:49:21.776678331 +0000 UTC m=+15849010.697255646.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.