

1,3-Dioxane, 5-bromo-5-nitro-

Other names:	5-Bromo-5-nitro-1,3-dioxane m-Dioxane, 5-bromo-5-nitro- 5-Brom-5-nitro-1,3-dioxan 5-Bromo-5-nitro-m-dioxane Bronidox Bronidox L
Inchi:	InChI=1S/C4H6BrNO4/c5-4(6(7)8)1-9-3-10-2-4/h1-3H2
InchiKey:	XVBRCOKDZVQYAY-UHFFFAOYSA-N
Formula:	C4H6BrNO4
SMILES:	O=[N+](O-)C1(Br)COCOC1
Mol. weight [g/mol]:	212.00
CAS:	30007-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-120.61	kJ/mol	Joback Method
hf	-304.76	kJ/mol	Joback Method
hfus	24.26	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.359		Crippen Method
mcvol	103.020	ml/mol	McGowan Method
pc	6018.58	kPa	Joback Method
tb	582.61	K	Joback Method
tc	858.49	K	Joback Method
tf	422.67	K	Joback Method
vc	0.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.21	J/mol×K	582.61	Joback Method
cpg	243.44	J/mol×K	628.59	Joback Method
cpg	252.78	J/mol×K	674.57	Joback Method

cpg	261.44	J/mol×K	720.55	Joback Method
cpg	269.65	J/mol×K	766.53	Joback Method
cpg	277.63	J/mol×K	812.51	Joback Method
cpg	285.60	J/mol×K	858.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30007477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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