Bronopol

Other names:	1,3-Propanediol, 2-bromo-2-nitro-
	Bronocot
	Onyxide 500
	2-Bromo-2-nitro-1,3-propanediol
	2-Bromo-2-nitropropane-1,3-diol
	Bronosol
	2-Nitro-2-bromo-1,3-propanediol
	2-Bromo-2-nitropropan-1,3-diol
	«beta»-Bromo-«beta»-nitrotrimethyleneglycol
	Bronopolu
	Bronotak
	Bioban
	Bronidiol
	Canguard 409
	Lexgard bronopol
	Myacide AS plus
	Myacide BT
	NSC 141021
	Myacide Pharma BP
Inchi:	InChI=1S/C3H6BrNO4/c4-3(1-6,2-7)5(8)9/h6-7H,1-2H2
InchiKey:	LVDKZNITIUWNER-UHFFFAOYSA-N
Formula:	C3H6BrNO4
SMILES:	O=[N+]([O-])C(Br)(CO)CO
Mol. weight [g/mol]:	199.99
CAS:	52-51-7

Physical Properties

Property code	Value	Unit	Source
gf	-246.55	kJ/mol	Joback Method
hf	-402.89	kJ/mol	Joback Method
hfus	20.93	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	-0.661		Crippen Method
mcvol	99.790	ml/mol	McGowan Method
pc	6696.65	kPa	Joback Method
tb	667.17	K	Joback Method

tc	874.85	K	Joback Method
tf	451.04	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.90	J/mol×K	667.17	Joback Method
cpg	236.91	J/mol×K	701.78	Joback Method
cpg	241.52	J/mol×K	736.40	Joback Method
cpg	245.78	J/mol×K	771.01	Joback Method
cpg	249.74	J/mol×K	805.62	Joback Method
cpg	253.43	J/mol×K	840.24	Joback Method
cpg	256.89	J/mol×K	874.85	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=C52517&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