2(3H)-Furanone, 3-bromodihydro-

Other names:	«alpha»-Bromo-«gamma»-butyrolactone
	2-Bromo-4-butyrolactone
	2-Bromo-«gamma»-butyrolactone
	«alpha»-Bromobutyric acid, «gamma»-lactone
	«alpha»-Bromobutyrolactone
	2-Bromo-4-butanolide
	2-Bromobutyrolactone
	3-Bromodihydro-2-furanone
	3-Bromodihydro-2(3H)-furanone
	Butyric acid, 2-bromo-4-hydroxy-, gamma-lactone
	3-Bromo-2-oxotetrahydrofuran
	NSC 56959
Inchi:	InChI=1S/C4H5BrO2/c5-3-1-2-7-4(3)6/h3H,1-2H2
InchiKey:	LFJJGHGXHXXDFT-UHFFFAOYSA-N
Formula:	C4H5BrO2
SMILES:	O=C1OCCC1Br
Mol. weight [g/mol]:	164.99
CAS:	5061-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-175.04	kJ/mol	Joback Method
hf	-308.78	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	39.95	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.697		Crippen Method
mcvol	81.300	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
tb	467.13	K	Joback Method
tc	710.18	K	Joback Method
tf	300.33	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.75	J/mol×K	467.13	Joback Method
cpg	158.59	J/mol×K	507.64	Joback Method
cpg	167.92	J/mol×K	548.15	Joback Method
cpg	176.75	J/mol×K	588.65	Joback Method
cpg	185.07	J/mol×K	629.16	Joback Method
cpg	192.87	J/mol×K	669.67	Joback Method
cpg	200.16	J/mol×K	710.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	0.80	NIST Webbook
tbrp	369.50 ± 0.50	K	0.70	NIST Webbook

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=C5061212&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume