

Mucobromic acid lactone

Other names:	3,4-dibromo-5-hydroxyfuran-2(5H)-one
Inchi:	InChI=1S/C4H2Br2O3/c5-1-2(6)4(8)9-3(1)7/h3,7H
InchiKey:	PKDBSOOYVOEUQR-UHFFFAOYSA-N
Formula:	C4H2Br2O3
SMILES:	O=C1OC(O)C(Br)=C1Br
Mol. weight [g/mol]:	257.87
CAS:	766-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-286.84	kJ/mol	Joback Method
hf	-399.84	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	0.863		Crippen Method
mcvol	100.370	ml/mol	McGowan Method
pc	7431.63	kPa	Joback Method
tb	634.59	K	Joback Method
tc	875.15	K	Joback Method
tf	446.75	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.45	J/molxK	634.59	Joback Method
cpg	194.26	J/molxK	674.68	Joback Method
cpg	199.70	J/molxK	714.78	Joback Method
cpg	204.75	J/molxK	754.87	Joback Method
cpg	209.42	J/molxK	794.97	Joback Method
cpg	213.70	J/molxK	835.06	Joback Method
cpg	217.58	J/molxK	875.15	Joback Method

Sources

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=C766381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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