Mucobromic acid

Other names:	2-Butenoic acid, 2,3-dibromo-4-oxo-, (Z)-
	Bromomucic acid
	Malealdehydic acid, dibromo-
	Mucobromic acid (2,3-dibromo-4-oxo-2-butenoic acid) (open form)
Inchi:	InChI=1S/C4H2Br2O3/c5-2(1-7)3(6)4(8)9/h1H,(H,8,9)/b3-2-
InchiKey:	NCNYEGJDGNOYJX-IHWYPQMZSA-N
Formula:	C4H2Br2O3
SMILES:	O=CC(Br)=C(Br)C(=O)O
Mol. weight [g/mol]:	257.87
CAS:	488-11-9

Physical Properties

Property code	Value	Unit	Source
gf	-290.70	kJ/mol	Joback Method
hf	-325.98	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	67.63	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.271		Crippen Method
mcvol	106.930	ml/mol	McGowan Method
pc	7267.82	kPa	Joback Method
tb	621.87	K	Joback Method
tc	843.79	K	Joback Method
tf	374.19	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.41	J/mol×K	621.87	Joback Method
cpg	187.11	J/mol×K	658.86	Joback Method
cpg	190.47	J/mol×K	695.84	Joback Method
cpg	193.53	J/mol×K	732.83	Joback Method
cpg	196.35	J/mol×K	769.81	Joback Method

cpg	198.96	J/mol×K	806.80	Joback Method
cpg	201.42	J/mol×K	843.79	Joback Method

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=C488119&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume