Bromoacetic acid

Other names:	2-Bromoacetic acid
	ALPHA-BROMOACETIC ACID
	Acetic acid, 2-bromo-
	Acide bromacetique
	Bromoethanoic acid
	CH2BrCOOH
	Kyselina bromoctova
	Monobromessigsaeure
	Monobromoacetic acid
	NSC 141
	To NTU
	UN 1938
	«alpha»-Bromoacetic acid
	«alpha»-Bromoethanoic acid
Inchi:	InChI=1S/C2H3BrO2/c3-1-2(4)5/h1H2,(H,4,5)
InchiKey:	KDPAWGWELVVRCH-UHFFFAOYSA-N
Formula:	C2H3O2Br
SMILES:	O=C(O)CBr
Mol. weight [g/mol]:	138.95
CAS:	79-08-3

Physical Properties

Property code	Value	Unit	Source
af	0.6447		Cheméo Relay (1.0)
gf	-285.46	kJ/mol	Joback Method
hf	-415.01	kJ/mol	Cheméo Relay (1.0)
hfus	11.91	kJ/mol	Joback Method
hsub	83.50 ± 3.00	kJ/mol	NIST Webbook
hvap	63.90	kJ/mol	Cheméo Relay (1.0)
ie	11.00	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
log10ws	0.38		Cheméo Relay (1.0)
logp	0.466		Crippen Method
mcvol	63.980	ml/mol	McGowan Method
pc	7109.36	kPa	Joback Method
tb	481.00	K	NIST Webbook
tb	481.20	K	NIST Webbook

tb	479.20	K	NIST Webbook
tc	707.56	K	Cheméo Relay (1.0)
tf	323.00	K	NIST Webbook
vc	0.228	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.14	J/mol×K	457.37	Joback Method
cpg	103.72	J/mol×K	489.66	Joback Method
cpg	107.09	J/mol×K	521.96	Joback Method
cpg	110.26	J/mol×K	554.25	Joback Method
cpg	113.25	J/mol×K	586.54	Joback Method
cpg	116.07	J/mol×K	618.84	Joback Method
cpg	118.71	J/mol×K	651.13	Joback Method
dvisc	0.0061078	Pa×s	311.94	Joback Method
dvisc	0.0151185	Pa×s	282.85	Joback Method
dvisc	0.0028801	Pa×s	341.02	Joback Method
dvisc	0.0015284	Pa×s	370.11	Joback Method
dvisc	0.0008896	Pa×s	399.20	Joback Method
dvisc	0.0005572	Pa×s	428.28	Joback Method
dvisc	0.0003705	Pa×s	457.37	Joback Method
hfust	13.90	kJ/mol	319.20	NIST Webbook
hvapt	57.20	kJ/mol	404.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.66739e+01
Coeff. B	-8.12419e+03
Coeff. C	-4.16026e+00
Coeff. D	2.25727e-06
Temperature range (K), min.	327.15
Temperature range (K), max.	481.15

Sources

Cheméo Relay (1.0):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1779
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79083&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1779
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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