

«alpha»-Bromoacrylic acid

Other names:	2-Bromoacrylic acid 2-Propenoic acid, 2-bromo-
Inchi:	InChI=1S/C3H3BrO2/c1-2(4)3(5)6/h1H2,(H,5,6)
InchiKey:	HMENQNSSJFLQOP-UHFFFAOYSA-N
Formula:	C3H3BrO2
SMILES:	C=C(Br)C(=O)O
Mol. weight [g/mol]:	150.96
CAS:	10443-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-197.75	kJ/mol	Joback Method
hf	-228.09	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	51.54	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.980		Crippen Method
mvol	73.770	ml/mol	McGowan Method
pc	6556.41	kPa	Joback Method
tb	476.81	K	Joback Method
tc	676.15	K	Joback Method
tf	278.40	K	Joback Method
vc	0.273	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.72	J/molxK	476.81	Joback Method
cpg	123.90	J/molxK	510.03	Joback Method
cpg	127.80	J/molxK	543.26	Joback Method
cpg	131.43	J/molxK	576.48	Joback Method
cpg	134.82	J/molxK	609.70	Joback Method
cpg	137.98	J/molxK	642.93	Joback Method
cpg	140.93	J/molxK	676.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10443659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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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