

2,3-Dibromobutyric acid

Other names:	«alpha», «beta»-Dibromobutyric acid «alpha», «beta»-Dibromo-n-butyric acid Butanoic acid, 2,3-dibromo-
Inchi:	InChI=1S/C4H6Br2O2/c1-2(5)3(6)4(7)8/h2-3H,1H3,(H,7,8)
InchiKey:	HESQKTULJLBDRF-UHFFFAOYSA-N
Formula:	C4H6Br2O2
SMILES:	CC(Br)C(Br)C(=O)O
Mol. weight [g/mol]:	245.90
CAS:	600-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-259.18	kJ/mol	Joback Method
hf	-348.60	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.618		Crippen Method
mcvol	109.660	ml/mol	McGowan Method
pc	5981.40	kPa	Joback Method
tb	568.41	K	Joback Method
tc	780.08	K	Joback Method
tf	335.19	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.20	J/molxK	568.41	Joback Method
cpg	227.31	J/molxK	744.80	Joback Method
cpg	222.80	J/molxK	709.52	Joback Method
cpg	217.96	J/molxK	674.24	Joback Method
cpg	212.77	J/molxK	638.97	Joback Method
cpg	207.19	J/molxK	603.69	Joback Method

cpg	231.51	J/mol×K	780.08	Joback Method
dvisc	0.0001628	Paxs	568.41	Joback Method
dvisc	0.0002493	Paxs	529.54	Joback Method
dvisc	0.0004083	Paxs	490.67	Joback Method
dvisc	0.0007280	Paxs	451.80	Joback Method
dvisc	0.0014472	Paxs	412.93	Joback Method
dvisc	0.0033188	Paxs	374.06	Joback Method
dvisc	0.0092262	Paxs	335.19	Joback Method

Sources

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=C600306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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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