

Acetic acid, dibromo-

Other names:	Dibromoacetic acid Dibromoethanoic acid
Inchi:	InChI=1S/C2H2Br2O2/c3-1(4)2(5)6/h1H,(H,5,6)
InchiKey:	SIEILFNCEFEENQ-UHFFFAOYSA-N
Formula:	C2H2Br2O2
SMILES:	O=C(O)C(Br)Br
Mol. weight [g/mol]:	217.84
CAS:	631-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-273.58	kJ/mol	Joback Method
hf	-302.04	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.187		Crippen Method
mcvol	81.480	ml/mol	McGowan Method
pc	8130.87	kPa	Joback Method
tb	523.09	K	Joback Method
tc	737.15	K	Joback Method
tf	327.65	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.96	J/mol×K	737.15	Joback Method
cpg	134.86	J/mol×K	701.47	Joback Method
cpg	132.58	J/mol×K	665.79	Joback Method
cpg	130.09	J/mol×K	630.12	Joback Method
cpg	127.38	J/mol×K	594.44	Joback Method
cpg	124.41	J/mol×K	558.77	Joback Method
cpg	121.18	J/mol×K	523.09	Joback Method

cps	124.68	J/mol×K	301.37	NIST Webbook
dvisc	0.0003891	Pa×s	490.52	Joback Method
dvisc	0.0006075	Pa×s	457.94	Joback Method
dvisc	0.0010154	Pa×s	425.37	Joback Method
dvisc	0.0018481	Pa×s	392.80	Joback Method
dvisc	0.0037485	Pa×s	360.22	Joback Method
dvisc	0.0087508	Pa×s	327.65	Joback Method
dvisc	0.0002635	Pa×s	523.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.20	K	2.10	NIST Webbook

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=C631641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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