Dibromoacetic acid

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

Physical Properties

Property code	Value	Unit	Source
af	0.6646		Cheméo Relay (1.0)
hf	-351.13	kJ/mol	Cheméo Relay (1.0)
hfus	13.67	kJ/mol	Joback Method
hvap	70.00	kJ/mol	Cheméo Relay (1.0)
ie	11.01	eV	Cheméo Relay (1.0)
log10ws	-0.07		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	81.480	ml/mol	McGowan Method
pc	8130.87	kPa	Joback Method
tb	497.17	K	Cheméo Relay (1.0)
tc	741.06	K	Cheméo Relay (1.0)
tf	326.18	K	Cheméo Relay (1.0)
vc	0.292	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

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

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C631641&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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