Propanoic acid, 2,3-dibromo-

Other names:	Propionic acid, 2,3-dibromo- «alpha»,«beta»-Dibromopropionic acid 2,3-Dibromopropanoic acid 2,3-Dibromopropionic acid
Inchi:	InChI=1S/C3H4Br2O2/c4-1-2(5)3(6)7/h2H,1H2,(H,6,7)
InchiKey:	ZMYAKSMZTVWUJB-UHFFFAOYSA-N
Formula:	C3H4Br2O2
SMILES:	O=C(O)C(Br)CBr
Mol. weight [g/mol]:	231.87
CAS:	600-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-265.16	kJ/mol	Joback Method
hf	-322.68	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.229		Crippen Method
mcvol	95.570	ml/mol	McGowan Method
pc	6886.93	kPa	Joback Method
tb	545.97	K	Joback Method
tc	756.57	K	Joback Method
tf	338.92	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.96	J/mol×K	545.97	Joback Method
cpg	164.56	J/mol×K	581.07	Joback Method
cpg	168.82	J/mol×K	616.17	Joback Method
cpg	172.77	J/mol×K	651.27	Joback Method
cpg	176.44	J/mol×K	686.37	Joback Method

cpg	179.84	J/mol×K	721.47	Joback Method
cpg	183.01	J/mol×K	756.57	Joback Method
dvisc	0.0073788	Pa×s	338.92	Joback Method
dvisc	0.0031123	Pa×s	373.43	Joback Method
dvisc	0.0015191	Pa×s	407.94	Joback Method
dvisc	0.0008293	Pa×s	442.44	Joback Method
dvisc	0.0004941	Pa×s	476.95	Joback Method
dvisc	0.0003157	Pa×s	511.46	Joback Method
dvisc	0.0002135	Pa×s	545.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	2.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C600055&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume