2-Bromopropionyl bromide

Other names: «alpha»-Bromopropionyl bromide
Propanoyl bromide, 2-bromo-
Inchi: InChI=1S/C3H4Br2O/c1-2(4)3(5)6/h2H,1H3
InchiKey: ILLHORFDXDLILE-UHFFFAOYSA-N
Formula: C3H4Br2O
SMILES: CC(Br)C(=O)Br
Mol. weight [g/mol]: 215.87
CAS: 563-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-128.34	kJ/mol	Joback Method
hf	-170.45	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.691		Crippen Method
mcvol	89.700	ml/mol	McGowan Method
pc	5944.56	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	680.62	K	Joback Method
tf	278.10	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.78	J/mol×K	453.79	Joback Method
cpg	136.32	J/mol×K	491.60	Joback Method
cpg	141.46	J/mol×K	529.40	Joback Method
cpg	146.21	J/mol×K	567.21	Joback Method
cpg	150.61	J/mol×K	605.01	Joback Method
cpg	154.67	J/mol×K	642.82	Joback Method
cpg	158.43	J/mol×K	680.62	Joback Method

dvisc	0.0037576	Pa×s	278.10	Joback Method
dvisc	0.0022894	Pa×s	307.38	Joback Method
dvisc	0.0015204	Pa×s	336.66	Joback Method
dvisc	0.0010781	Pa×s	365.95	Joback Method
dvisc	0.0008044	Pa×s	395.23	Joback Method
dvisc	0.0006249	Pa×s	424.51	Joback Method
dvisc	0.0005016	Pa×s	453.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	322.20	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C563768&Units=SI
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

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