

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

Physical Properties

Property code	Value	Unit	Source
hf	-192.49	kJ/mol	Cheméo Relay (1.0)
hfus	12.17	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Cheméo Relay (1.0)
ie	10.26	eV	Cheméo Relay (1.0)
logp	1.691		Crippen Method
mcvol	89.700	ml/mol	McGowan Method
tb	426.20	K	NIST Webbook
tf	294.17	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.78	J/mol×K	453.79	Joback Method
cpg	158.43	J/mol×K	680.62	Joback Method
cpg	154.67	J/mol×K	642.82	Joback Method
cpg	150.61	J/mol×K	605.01	Joback Method
cpg	146.21	J/mol×K	567.21	Joback Method
cpg	141.46	J/mol×K	529.40	Joback Method
cpg	136.32	J/mol×K	491.60	Joback Method
dvisc	0.0010781	Pa×s	365.95	Joback Method
dvisc	0.0005016	Pa×s	453.79	Joback Method
dvisc	0.0006249	Pa×s	424.51	Joback Method
dvisc	0.0008044	Pa×s	395.23	Joback Method
dvisc	0.0037576	Pa×s	278.10	Joback Method

dvisc	0.0015204	Pa×s	336.66	Joback Method
dvisc	0.0022894	Pa×s	307.38	Joback Method

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C563768&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

cpg:	Ideal gas 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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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