

1-Propanol, 2,3-dibromo-

Other names:	1,2-Dibromohydrin 1,2-Dibromopropan-3-ol 1-Propanol, 2,3-dibromo- 2,3-Dibromo-1-propanol 2,3-Dibromopropanol 2,3-dibromopropan-1-ol Brominex 257 DBP DBP (flame retardant) NCI-C55436 NSC 6203 USAF DO-42 «beta»-Dibromohydrin
Inchi:	InChI=1S/C3H6Br2O/c4-1-3(5)2-6/h3,6H,1-2H2
InchiKey:	QWVCIORZLNBIIC-UHFFFAOYSA-N
Formula:	C3H6Br2O
SMILES:	OCC(Br)CBr
Mol. weight [g/mol]:	217.89

Physical Properties

Property code	Value	Unit	Source
hf	-221.30	kJ/mol	Cheméo Relay (1.0)
hfus	14.66	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Cheméo Relay (1.0)
log10ws	-0.55		Cheméo Relay (1.0)
logp	1.137		Crippen Method
mcvol	94.000	ml/mol	McGowan Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	487.97	K	Cheméo Relay (1.0)
tf	260.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.18	J/mol×K	492.10	Joback Method
cpg	183.24	J/mol×K	693.60	Joback Method
cpg	179.28	J/mol×K	660.02	Joback Method
cpg	175.07	J/mol×K	626.43	Joback Method
cpg	170.57	J/mol×K	592.85	Joback Method
cpg	165.78	J/mol×K	559.27	Joback Method
cpg	160.65	J/mol×K	525.68	Joback Method
dvisc	0.0012488	Pa×s	390.54	Joback Method
dvisc	0.0002669	Pa×s	492.10	Joback Method
dvisc	0.0004138	Pa×s	458.25	Joback Method
dvisc	0.0006879	Pa×s	424.40	Joback Method
dvisc	0.0172793	Pa×s	288.99	Joback Method
dvisc	0.0025389	Pa×s	356.69	Joback Method
dvisc	0.0059899	Pa×s	322.84	Joback Method
hvapt	57.30	kJ/mol	411.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C96139&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

Cheméo Relay (1.0):

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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