

2-PROPANOL, 1-BROMO-

Other names:	1-Bromo-2-propanol 2-Hydroxy-2-methylethyl bromide 2-Hydroxypropyl bromide Propylene bromohydrin 1-Bromo-2-hydroxypropane 1-bromopropan-2-ol
Inchi:	InChI=1S/C3H7BrO/c1-3(5)2-4/h3,5H,2H2,1H3
InchiKey:	WEGOLYBUWCMMMY-UHFFFAOYSA-N
Formula:	C3H7BrO
SMILES:	CC(O)CBr
Mol. weight [g/mol]:	138.99

Physical Properties

Property code	Value	Unit	Source
af	0.5794		Cheméo Relay (1.0)
gf	-150.56	kJ/mol	Joback Method
hf	-287.32	kJ/mol	Cheméo Relay (1.0)
hfus	9.38	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Cheméo Relay (1.0)
ie	10.38	eV	Cheméo Relay (1.0)
log10ws	0.17		Cheméo Relay (1.0)
logp	0.762		Crippen Method
mcvol	76.500	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	419.70	K	NIST Webbook
tc	615.14	K	Cheméo Relay (1.0)
tf	201.00	K	Cheméo Relay (1.0)
vc	0.283	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.15	J/mol×K	425.94	Joback Method
cpg	135.04	J/mol×K	456.76	Joback Method

cpg	140.63	J/mol×K	487.57	Joback Method
cpg	145.95	J/mol×K	518.39	Joback Method
cpg	151.01	J/mol×K	549.21	Joback Method
cpg	155.81	J/mol×K	580.03	Joback Method
cpg	160.37	J/mol×K	610.84	Joback Method
dvisc	0.0745644	Pa×s	229.19	Joback Method
dvisc	0.0176820	Pa×s	261.98	Joback Method
dvisc	0.0057755	Pa×s	294.77	Joback Method
dvisc	0.0023601	Pa×s	327.56	Joback Method
dvisc	0.0011351	Pa×s	360.36	Joback Method
dvisc	0.0006168	Pa×s	393.15	Joback Method
dvisc	0.0003682	Pa×s	425.94	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19686738&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
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

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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