

1-Bromo-2-butanol

Inchi:	InChI=1S/C4H9BrO/c1-2-4(6)3-5/h4,6H,2-3H2,1H3
InchiKey:	DMRXISNUOWIOKV-UHFFFAOYSA-N
Formula:	C4H9BrO
SMILES:	CCC(O)CBr
Mol. weight [g/mol]:	153.02
CAS:	2482-57-7

Physical Properties

Property code	Value	Unit	Source
gf	-142.14	kJ/mol	Joback Method
hf	-257.07	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.152		Crippen Method
mcvol	90.590	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
tb	448.82	K	Joback Method
tc	632.13	K	Joback Method
tf	240.46	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.81	J/molxK	632.13	Joback Method
cpg	165.40	J/molxK	448.82	Joback Method
cpg	172.61	J/molxK	479.37	Joback Method
cpg	179.48	J/molxK	509.92	Joback Method
cpg	186.02	J/molxK	540.48	Joback Method
cpg	192.25	J/molxK	571.03	Joback Method
cpg	198.17	J/molxK	601.58	Joback Method
dvisc	0.0002989	Paxs	448.82	Joback Method
dvisc	0.0580626	Paxs	240.46	Joback Method

dvisc	0.0138627	Paxs	275.19	Joback Method
dvisc	0.0045625	Paxs	309.91	Joback Method
dvisc	0.0018786	Paxs	344.64	Joback Method
dvisc	0.0009099	Paxs	379.37	Joback Method
dvisc	0.0004977	Paxs	414.09	Joback Method
hvapt	58.40	kJ/mol	357.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2482577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	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
hvapt:	Enthalpy of vaporization at a given temperature
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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