

1-Butanol, 2,3-dimethyl-

Inchi:	InChI=1S/C6H14O/c1-5(2)6(3)4-7/h5-7H,4H2,1-3H3
InchiKey:	SXSWMAUXEHKFGX-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CC(C)C(C)CO
Mol. weight [g/mol]:	102.17
CAS:	20281-85-0

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-329.96	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.271		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	417.70	K	NIST Webbook
tc	596.11	K	Joback Method
tf	188.20	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.81	J/molxK	427.98	Joback Method
cpg	217.90	J/molxK	456.00	Joback Method
cpg	227.60	J/molxK	484.02	Joback Method
cpg	236.93	J/molxK	512.04	Joback Method
cpg	245.89	J/molxK	540.06	Joback Method
cpg	254.50	J/molxK	568.09	Joback Method
cpg	262.76	J/molxK	596.11	Joback Method
dvisc	0.6544822	Paxs	188.20	Joback Method
dvisc	0.0545090	Paxs	228.16	Joback Method

dvisc	0.0095238	Paxs	268.13	Joback Method
dvisc	0.0026164	Paxs	308.09	Joback Method
dvisc	0.0009671	Paxs	348.05	Joback Method
dvisc	0.0004388	Paxs	388.02	Joback Method
dvisc	0.0002307	Paxs	427.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20281850&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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