

3-methylbutane-1,2-diol

Inchi:	InChI=1S/C5H12O2/c1-4(2)5(7)3-6/h4-7H,3H2,1-2H3
InchiKey:	HJJZIMFAIMUSBW-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CC(C)C(O)CO
Mol. weight [g/mol]:	104.15
CAS:	50468-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-287.30	kJ/mol	Joback Method
hf	-461.55	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.004		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	461.15 ± 2.00	K	NIST Webbook
tb	473.02 ± 3.00	K	NIST Webbook
tc	661.20	K	Joback Method
tf	237.75	K	Joback Method
vc	0.342	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.59	J/mol×K	497.28	Joback Method
cpg	221.48	J/mol×K	524.60	Joback Method
cpg	229.06	J/mol×K	551.92	Joback Method
cpg	236.33	J/mol×K	579.24	Joback Method
cpg	243.30	J/mol×K	606.56	Joback Method
cpg	249.98	J/mol×K	633.88	Joback Method
cpg	256.38	J/mol×K	661.20	Joback Method
dvisc	1.1462269	Paxs	237.75	Joback Method

dvisc	0.0710068	Paxs	281.00	Joback Method
dvisc	0.0092386	Paxs	324.26	Joback Method
dvisc	0.0019427	Paxs	367.51	Joback Method
dvisc	0.0005673	Paxs	410.77	Joback Method
dvisc	0.0002095	Paxs	454.02	Joback Method
dvisc	0.0000920	Paxs	497.28	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50468229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
h_{vap}:	Enthalpy of vaporization at standard conditions
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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