

2-methylbutane-2,3-diol

Inchi:	InChI=1S/C5H12O2/c1-4(6)5(2,3)7/h4,6-7H,1-3H3
InchiKey:	IDEOPBXRUBNYBN-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CC(O)C(C)(C)O
Mol. weight [g/mol]:	104.15
CAS:	5396-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-282.02	kJ/mol	Joback Method
hf	-465.02	kJ/mol	Joback Method
hfus	5.95	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.138		Crippen Method
mvol	93.050	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	446.65 ± 3.00	K	NIST Webbook
tb	450.65 ± 3.00	K	NIST Webbook
tb	446.15 ± 4.00	K	NIST Webbook
tc	664.19	K	Joback Method
tf	255.17	K	Joback Method
vc	0.337	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.81	J/mol×K	494.49	Joback Method
cpg	225.13	J/mol×K	522.77	Joback Method
cpg	233.03	J/mol×K	551.06	Joback Method
cpg	240.53	J/mol×K	579.34	Joback Method
cpg	247.63	J/mol×K	607.62	Joback Method
cpg	254.37	J/mol×K	635.91	Joback Method
cpg	260.76	J/mol×K	664.19	Joback Method

dvisc	0.4952678	Paxs	255.17	Joback Method
dvisc	0.0456841	Paxs	295.06	Joback Method
dvisc	0.0074338	Paxs	334.94	Joback Method
dvisc	0.0017803	Paxs	374.83	Joback Method
dvisc	0.0005613	Paxs	414.72	Joback Method
dvisc	0.0002167	Paxs	454.60	Joback Method
dvisc	0.0000975	Paxs	494.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5396587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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