

2-methylbutanol-d-9

Inchi:	InChI=1S/C5H12O/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3/i1D3,2D3,3D2,5D
InchiKey:	QPRQEDXDYOZYLA-APXHDBETSA-N
Formula:	C5H3D9O
SMILES:	CCC(C)CO
Mol. weight [g/mol]:	97.20

Physical Properties

Property code	Value	Unit	Source
gf	-148.04	kJ/mol	Joback Method
hf	-304.04	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.025		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
ripol	1207.00		NIST Webbook
ripol	1207.00		NIST Webbook
tb	405.54	K	Joback Method
tc	570.76	K	Joback Method
tf	191.93	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.82	J/molxK	405.54	Joback Method
cpg	178.43	J/molxK	433.08	Joback Method
cpg	186.73	J/molxK	460.61	Joback Method
cpg	194.72	J/molxK	488.15	Joback Method
cpg	202.42	J/molxK	515.68	Joback Method
cpg	209.82	J/molxK	543.22	Joback Method
cpg	216.94	J/molxK	570.76	Joback Method
dvisc	0.3005917	Paxs	191.93	Joback Method

dvisc	0.0379452	Paxs	227.53	Joback Method
dvisc	0.0083860	Paxs	263.13	Joback Method
dvisc	0.0026559	Paxs	298.74	Joback Method
dvisc	0.0010745	Paxs	334.34	Joback Method
dvisc	0.0005174	Paxs	369.94	Joback Method
dvisc	0.0002833	Paxs	405.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322524&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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