

2-methylbutanol-d-3

Inchi: InChI=1S/C5H12O/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3/i1D3
InchiKey: QPRQEDXDYOZYLA-FIBGUPNXSA-N
Formula: C5H9D3O
SMILES: CCC(C)CO
Mol. weight [g/mol]: 91.17

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	1209.00		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/mol×K	405.54	Joback Method
cpg	178.43	J/mol×K	433.08	Joback Method
cpg	186.73	J/mol×K	460.61	Joback Method
cpg	194.72	J/mol×K	488.15	Joback Method
cpg	202.42	J/mol×K	515.68	Joback Method
cpg	209.82	J/mol×K	543.22	Joback Method
cpg	216.94	J/mol×K	570.76	Joback Method
dvisc	0.3005917	Pa×s	191.93	Joback Method
dvisc	0.0379452	Pa×s	227.53	Joback Method

dvisc	0.0083860	Pa×s	263.13	Joback Method
dvisc	0.0026559	Pa×s	298.74	Joback Method
dvisc	0.0010745	Pa×s	334.34	Joback Method
dvisc	0.0005174	Pa×s	369.94	Joback Method
dvisc	0.0002833	Pa×s	405.54	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=R322519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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