

4-Propan-2-yloxy-2-butanol

Inchi:	InChI=1S/C7H16O2/c1-6(2)9-5-4-7(3)8/h6-8H,4-5H2,1-3H3
InchiKey:	IVTACLGUUXBTMN-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CC(O)CCOC(C)C
Mol. weight [g/mol]:	132.20

Physical Properties

Property code	Value	Unit	Source
gf	-238.64	kJ/mol	Joback Method
hf	-482.82	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.182		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
ripol	1717.00		NIST Webbook
ripol	1717.00		NIST Webbook
tb	473.28	K	Joback Method
tc	640.32	K	Joback Method
tf	221.70	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.70	J/mol×K	473.28	Joback Method
cpg	322.87	J/mol×K	612.48	Joback Method
cpg	313.37	J/mol×K	584.64	Joback Method
cpg	303.51	J/mol×K	556.80	Joback Method
cpg	293.28	J/mol×K	528.96	Joback Method
cpg	282.68	J/mol×K	501.12	Joback Method
cpg	332.00	J/mol×K	640.32	Joback Method
dvisc	0.0001445	Pa×s	473.28	Joback Method

dvisc	0.0002615	Pa×s	431.35	Joback Method
dvisc	0.0005376	Pa×s	389.42	Joback Method
dvisc	0.0013151	Pa×s	347.49	Joback Method
dvisc	0.0041121	Pa×s	305.56	Joback Method
dvisc	0.0184782	Pa×s	263.63	Joback Method
dvisc	0.1465922	Pa×s	221.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R634847&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

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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