1-Butanol, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-

Other names: 4-(2-Tetrahydropyranyloxy)butan-1-ol
Inchi: InChI=1S/C9H18O3/c10-6-2-4-8-12-9-5-1-3-7-11-9/h9-10H,1-8H2
InchiKey: MAASHSYTIKTSSQ-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: OCCCCOC1CCCCO1
Mol. weight [g/mol]: 174.24
CAS: 51326-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-278.59	kJ/mol	Joback Method
hf	-591.22	kJ/mol	Joback Method
hfus	24.16	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.302		Crippen Method
mcvol	144.420	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1465.00		NIST Webbook
tb	566.42	K	Joback Method
tc	752.93	K	Joback Method
tf	308.19	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.88	J/mol×K	566.42	Joback Method
cpg	393.64	J/mol×K	597.50	Joback Method
cpg	407.71	J/mol×K	628.59	Joback Method
cpg	421.09	J/mol×K	659.67	Joback Method

cpg	433.80	J/mol×K	690.76	Joback Method
cpg	445.84	J/mol×K	721.84	Joback Method
cpg	457.22	J/mol×K	752.93	Joback Method
dvisc	0.0135363	Pa×s	308.19	Joback Method
dvisc	0.0035720	Pa×s	351.23	Joback Method
dvisc	0.0012608	Pa×s	394.27	Joback Method
dvisc	0.0005463	Pa×s	437.30	Joback Method
dvisc	0.0002749	Pa×s	480.34	Joback Method
dvisc	0.0001549	Pa×s	523.38	Joback Method
dvisc	0.0000953	Pa×s	566.42	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51326513&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume