3-OH-benzyl

Inchi: InChI=1S/C7H7O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H2
InchiKey: OKXJJSDTQZSGLY-UHFFFAOYSA-N
Formula: C7H7O
SMILES: [CH2]c1cccc(O)c1
Mol. weight [g/mol]: 107.13
CAS: 155174-22-4

Physical Properties

Property code	Value	Unit	Source
affp	885.50	kJ/mol	NIST Webbook
basg	853.00	kJ/mol	NIST Webbook
gf	18.23	kJ/mol	Joback Method
hf	-72.78	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	46.32	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.574		Crippen Method
mcvol	89.450	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
tb	466.16	K	Joback Method
tc	691.87	K	Joback Method
tf	323.16	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.64	J/mol×K	466.16	Joback Method
cpg	187.45	J/mol×K	503.78	Joback Method
cpg	196.30	J/mol×K	541.40	Joback Method
cpg	204.30	J/mol×K	579.01	Joback Method
cpg	211.56	J/mol×K	616.63	Joback Method
cpg	218.18	J/mol×K	654.25	Joback Method
cpg	224.27	J/mol×K	691.87	Joback Method

dvisc	0.0038840	Pa×s	323.16	Joback Method
dvisc	0.0020261	Pa×s	346.99	Joback Method
dvisc	0.0011492	Pa×s	370.83	Joback Method
dvisc	0.0006980	Pa×s	394.66	Joback Method
dvisc	0.0004487	Pa×s	418.49	Joback Method
dvisc	0.0003025	Pa×s	442.33	Joback Method
dvisc	0.0002124	Pa×s	466.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C155174224&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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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