4-(1-Hydroxyethyl)benzaldehyde

Inchi: InChI=1S/C9H10O2/c1-7(11)9-4-2-8(6-10)3-5-9/h2-7,11H,1H3
InchiKey: KPQCYFPPETYXOG-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: CC(O)c1ccc(C=O)cc1
Mol. weight [g/mol]: 150.17
CAS: 80463-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-111.10	kJ/mol	Joback Method
hf	-247.12	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.552		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	1291.00		NIST Webbook
ripol	1792.00		NIST Webbook
tb	577.38	K	Joback Method
tc	781.10	K	Joback Method
tf	317.95	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.14	J/mol×K	577.38	Joback Method
cpg	292.39	J/mol×K	611.33	Joback Method
cpg	302.03	J/mol×K	645.29	Joback Method
cpg	311.08	J/mol×K	679.24	Joback Method
cpg	319.57	J/mol×K	713.19	Joback Method
cpg	327.51	J/mol×K	747.15	Joback Method
cpg	334.94	J/mol×K	781.10	Joback Method

dvisc	0.0085877	Pa×s	317.95	Joback Method
dvisc	0.0026829	Pa×s	361.19	Joback Method
dvisc	0.0010749	Pa×s	404.43	Joback Method
dvisc	0.0005139	Pa×s	447.66	Joback Method
dvisc	0.0002798	Pa×s	490.90	Joback Method
dvisc	0.0001681	Pa×s	534.14	Joback Method
dvisc	0.0001090	Pa×s	577.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80463214&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

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