4-(2-hydroxy-2-propyl)benzaldehyde

Inchi: InChI=1S/C10H12O2/c1-10(2,12)9-5-3-8(7-11)4-6-9/h3-7,12H,1-2H3
InchiKey: RCUMJJBGXUQSOF-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)(O)c1ccc(C=O)cc1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
gf	-97.40	kJ/mol	Joback Method
hf	-271.23	kJ/mol	Joback Method
hfus	14.27	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.726		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1365.00		NIST Webbook
tb	597.47	K	Joback Method
tc	805.63	K	Joback Method
tf	346.64	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.36	J/mol×K	597.47	Joback Method
cpg	380.85	J/mol×K	770.93	Joback Method
cpg	372.32	J/mol×K	736.24	Joback Method
cpg	363.15	J/mol×K	701.55	Joback Method
cpg	353.30	J/mol×K	666.86	Joback Method
cpg	342.72	J/mol×K	632.16	Joback Method
cpg	388.79	J/mol×K	805.63	Joback Method
dvisc	0.0000899	Pa×s	597.47	Joback Method
dvisc	0.0001377	Pa×s	555.66	Joback Method

dvisc	0.0002261	Pa×s	513.86	Joback Method
dvisc	0.0004053	Pa×s	472.06	Joback Method
dvisc	0.0008138	Pa×s	430.25	Joback Method
dvisc	0.0018986	Pa×s	388.44	Joback Method
dvisc	0.0054341	Pa×s	346.64	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=R342766&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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