3-Hydroxyperillaldehyde

Inchi: InChI=1S/C10H14O2/c1-7(2)9-4-3-8(6-11)5-10(9)12/h5-6,9-10,12H,1,3-4H2,2H3
InchiKey: CGYLWHVYZDSTDR-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: C=C(C)C1CCC(C=O)=CC1O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-86.66	kJ/mol	Joback Method
hf	-291.61	kJ/mol	Joback Method
hfus	19.18	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.459		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
tb	584.62	K	Joback Method
tc	783.90	K	Joback Method
tf	305.98	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.59	J/mol×K	584.62	Joback Method
cpg	366.11	J/mol×K	617.83	Joback Method
cpg	378.88	J/mol×K	651.05	Joback Method
cpg	390.93	J/mol×K	684.26	Joback Method
cpg	402.27	J/mol×K	717.47	Joback Method
cpg	412.94	J/mol×K	750.69	Joback Method
cpg	422.94	J/mol×K	783.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514793&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

cpg:	Ideal gas heat capacity
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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