

3-(4-Hydroxyphenyl)propanal

Inchi:	InChI=1S/C9H10O2/c10-7-1-2-8-3-5-9(11)6-4-8/h3-7,11H,1-2H2
InchiKey:	REEQXZCFSBLNDH-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	O=CCc1ccc(O)cc1
Mol. weight [g/mol]:	150.17
CAS:	20238-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-116.83	kJ/mol	Joback Method
hf	-255.45	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.524		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
rinpol	1489.50		NIST Webbook
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tb	561.28	K	Joback Method
tc	786.65	K	Joback Method
tf	371.33	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.99	J/molxK	561.28	Joback Method
cpg	294.18	J/molxK	598.84	Joback Method
cpg	304.55	J/molxK	636.40	Joback Method
cpg	314.17	J/molxK	673.96	Joback Method
cpg	323.12	J/molxK	711.53	Joback Method
cpg	331.49	J/molxK	749.09	Joback Method
cpg	339.35	J/molxK	786.65	Joback Method

dvisc	0.0022311	Paxs	371.33	Joback Method
dvisc	0.0009783	Paxs	402.99	Joback Method
dvisc	0.0004837	Paxs	434.65	Joback Method
dvisc	0.0002632	Paxs	466.31	Joback Method
dvisc	0.0001547	Paxs	497.96	Joback Method
dvisc	0.0000969	Paxs	529.62	Joback Method
dvisc	0.0000640	Paxs	561.28	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=C20238839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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