Paroxypropione

Other names:

1-(4-hydroxyphenyl)-1-propanone
1-(4-hydroxyphenyl)propan-1-one
1-(p-Hydroxyphenyl)-1-Propanone
1-Propanone, 1-(4-hydroxyphenyl)-
4'-hydroxypropiophenone
4-Hydroxypropiophenon
4-Hydroxypropiophenone
4-Propanoylphenol
4-Propionylphenol
B 360
Bio-Fren
Ethyl p-hydroxyphenyl ketone
Frenantol
Frenohypon
Frenon
Frenormon
H-365
Hydroxypropiophenone
Hypophenon
Hypostat
Ibiopopp
Mepal
NSC-2834
P.O.P.
POP
Paroxon
Paroxypropion
Possipion
Possipione
Profenone
Propiophenone, 4'-hydroxy-
Proxiphenon
Sterofenon
USAF EK-3302
p-Hydroxyphenyl-1-propanone
p-Oxypropiophenone
p-Propionylphenol
p-Propiophenol
p-hydroxypropiophenone
para-Hydroxypropiophenone

Inchi:	InChI=1S/C9H10O2/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6,10H,2H2,1H3
InchiKey:	RARSHUDCJQSEFJ-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CCC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	150.17
CAS:	70-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-146.23	kJ/mol	Joback Method
hf	-282.45	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.985		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	566.49	K	Joback Method
tc	797.35	K	Joback Method
tf	421.60	K	Thermochemistry of 4-HOC6H4COR (R = H, CH3, C2H5, n-C3H7, n-C4H9, n-C5H11, and n-C6H13) compounds
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.64	J/mol×K	566.49	Joback Method
cpg	293.13	J/mol×K	604.97	Joback Method
cpg	303.76	J/mol×K	643.44	Joback Method
cpg	313.62	J/mol×K	681.92	Joback Method
cpg	322.80	J/mol×K	720.40	Joback Method
cpg	331.37	J/mol×K	758.87	Joback Method
cpg	339.41	J/mol×K	797.35	Joback Method
dvisc	0.0017635	Pa×s	379.26	Joback Method
dvisc	0.0007989	Pa×s	410.46	Joback Method

dvisc	0.0004047	Pa×s	441.67	Joback Method
dvisc	0.0002243	Pa×s	472.88	Joback Method
dvisc	0.0001337	Pa×s	504.08	Joback Method
dvisc	0.0000847	Pa×s	535.28	Joback Method
dvisc	0.0000564	Pa×s	566.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of 4-HOC6H4COR (R = H, CH3, C2H5, n-C3H7, n-C4H9, n-C5H11, and n-C6H13) compounds:	https://www.doi.org/10.1016/j.jct.2016.09.026
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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