

2-Hydroxy-1-(4-methoxyphenyl)propan-1-one

Inchi:	InChI=1S/C10H12O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-7,11H,1-2H3
InchiKey:	GTROJNGJJKJMDO-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccc(C(=O)C(C)O)cc1
Mol. weight [g/mol]:	180.20
CAS:	15482-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-237.08	kJ/mol	Joback Method
hf	-426.98	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.259		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1556.40		NIST Webbook
tb	627.89	K	Joback Method
tc	831.09	K	Joback Method
tf	359.38	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.72	J/molxK	627.89	Joback Method
cpg	361.92	J/molxK	661.76	Joback Method
cpg	372.47	J/molxK	695.62	Joback Method
cpg	382.39	J/molxK	729.49	Joback Method
cpg	391.69	J/molxK	763.36	Joback Method
cpg	400.38	J/molxK	797.22	Joback Method
cpg	408.47	J/molxK	831.09	Joback Method
dvisc	0.0033905	Paxs	359.38	Joback Method

dvisc	0.0012040	Paxs	404.13	Joback Method
dvisc	0.0005256	Paxs	448.88	Joback Method
dvisc	0.0002667	Paxs	493.63	Joback Method
dvisc	0.0001515	Paxs	538.39	Joback Method
dvisc	0.0000938	Paxs	583.14	Joback Method
dvisc	0.0000622	Paxs	627.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15482287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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