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

Inchi: InChI=1S/C10H12O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-6,10,12H,1-2H3
InchiKey: UVVXGUZSUNRWQG-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COc1ccc(C(O)C(C)=O)cc1
Mol. weight [g/mol]: 180.20
CAS: 15482-29-8

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	-1.82		Crippen Method
logp	1.318		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1678.20		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/mol×K	627.89	Joback Method
cpg	400.38	J/mol×K	797.22	Joback Method
cpg	391.69	J/mol×K	763.36	Joback Method
cpg	382.39	J/mol×K	729.49	Joback Method
cpg	372.47	J/mol×K	695.62	Joback Method
cpg	361.92	J/mol×K	661.76	Joback Method
cpg	408.47	J/mol×K	831.09	Joback Method
dvisc	0.0000622	Pa×s	627.89	Joback Method

dvisc	0.0000938	Pa×s	583.14	Joback Method
dvisc	0.0001515	Pa×s	538.39	Joback Method
dvisc	0.0002667	Pa×s	493.63	Joback Method
dvisc	0.0005256	Pa×s	448.88	Joback Method
dvisc	0.0012040	Pa×s	404.13	Joback Method
dvisc	0.0033905	Pa×s	359.38	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=C15482298&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