2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-

Other names: 1-Hydroxy-3-(4-hydroxy-3-methoxyphenyl)propan-2-one
Inchi: InChI=1S/C10H12O4/c1-14-10-5-7(2-3-9(10)13)4-8(12)6-11/h2-3,5,11,13H,4,6H2,1H3
InchiKey: CSQGINGXEBQJPA-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: COc1cc(CC(=O)CO)ccc1O
Mol. weight [g/mol]: 196.20
CAS: 4899-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-389.26	kJ/mol	Joback Method
hf	-599.01	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.505		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1735.70		NIST Webbook
rinpol	1735.70		NIST Webbook
tb	708.95	K	Joback Method
tc	917.59	K	Joback Method
tf	486.10	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.98	J/mol×K	708.95	Joback Method
cpg	404.64	J/mol×K	743.72	Joback Method
cpg	413.76	J/mol×K	778.50	Joback Method
cpg	422.39	J/mol×K	813.27	Joback Method
cpg	430.57	J/mol×K	848.04	Joback Method
cpg	438.35	J/mol×K	882.82	Joback Method

cpg	445.79	J/mol×K	917.59	Joback Method
dvisc	0.0002007	Pa×s	486.10	Joback Method
dvisc	0.0000856	Pa×s	523.24	Joback Method
dvisc	0.0000409	Pa×s	560.38	Joback Method
dvisc	0.0000214	Pa×s	597.52	Joback Method
dvisc	0.0000121	Pa×s	634.67	Joback Method
dvisc	0.0000073	Pa×s	671.81	Joback Method
dvisc	0.0000046	Pa×s	708.95	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4899745&Units=SI

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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