4-(3,4-dihydroxyphenyl)-butan-2-one

Inchi: InChI=1S/C10H12O3/c1-7(11)2-3-8-4-5-9(12)10(13)6-8/h4-6,12-13H,2-3H2,1H3
InchiKey: QIZQZQCADPIVCI-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CC(=O)CCc1ccc(O)c(O)c1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-292.43	kJ/mol	Joback Method
hf	-480.40	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.619		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	1749.00		NIST Webbook
tb	669.99	K	Joback Method
tc	905.37	K	Joback Method
tf	502.25	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.16	J/mol×K	669.99	Joback Method
cpg	382.81	J/mol×K	709.22	Joback Method
cpg	392.80	J/mol×K	748.45	Joback Method
cpg	402.26	J/mol×K	787.68	Joback Method
cpg	411.36	J/mol×K	826.91	Joback Method
cpg	420.21	J/mol×K	866.14	Joback Method
cpg	428.97	J/mol×K	905.37	Joback Method
dvisc	0.0000813	Pa×s	502.25	Joback Method
dvisc	0.0000408	Pa×s	530.21	Joback Method

dvisc	0.0000220	Pa×s	558.16	Joback Method
dvisc	0.0000126	Pa×s	586.12	Joback Method
dvisc	0.0000075	Pa×s	614.08	Joback Method
dvisc	0.0000047	Pa×s	642.03	Joback Method
dvisc	0.0000031	Pa×s	669.99	Joback Method

Sources

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=R420549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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