1-(2,3-dihydro-5-benzofuranyl)-ethanone

Inchi: InChI=1S/C10H10O2/c1-7(11)8-2-3-10-9(6-8)4-5-12-10/h2-3,6H,4-5H2,1H3
InchiKey: MMVUJVASBDVNGJ-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: CC(=O)c1ccc2c(c1)CCO2
Mol. weight [g/mol]: 162.19
CAS: 90843-31-5

Physical Properties

Property code	Value	Unit	Source
affp	902.60	kJ/mol	NIST Webbook
basg	870.70	kJ/mol	NIST Webbook
gf	-20.11	kJ/mol	Joback Method
hf	-187.58	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.824		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	557.07	K	Joback Method
tc	789.22	K	Joback Method
tf	352.60	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.14	J/mol×K	557.07	Joback Method
cpg	301.05	J/mol×K	595.76	Joback Method
cpg	313.03	J/mol×K	634.45	Joback Method
cpg	324.12	J/mol×K	673.14	Joback Method
cpg	334.41	J/mol×K	711.84	Joback Method
cpg	343.96	J/mol×K	750.53	Joback Method
cpg	352.83	J/mol×K	789.22	Joback Method

dvisc	0.0021013	Pa×s	352.60	Joback Method
dvisc	0.0014854	Pa×s	386.68	Joback Method
dvisc	0.0011107	Pa×s	420.76	Joback Method
dvisc	0.0008675	Pa×s	454.83	Joback Method
dvisc	0.0007013	Pa×s	488.91	Joback Method
dvisc	0.0005829	Pa×s	522.99	Joback Method
dvisc	0.0004955	Pa×s	557.07	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=C90843315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.