Ethanone, 1-(2,3-dihydro-1,4-benzodioxin-6-yl)-

Other names: 6-Acetyl-1,4-benzodioxane
6-Acetyl-1,4-benzodioxan
1,4-Benzodioxin, ethanone deriv.
Ketone, 1,4-benzodioxan-6-yl methyl
1,4-Benzodioxan-6-yl methyl ketone
1-(2,3-Dihydro-benzo[1,4]dioxin-6-yl)-ethanone
6-Acetylbenzodioxan

Inchi: InChI=1S/C10H10O3/c1-7(11)8-2-3-9-10(6-8)13-5-4-12-9/h2-3,6H,4-5H2,1H3

InchiKey: HGVWMTAIIYNQSI-UHFFFAOYSA-N

Formula: C10H10O3

SMILES: CC(=O)c1ccc2c(c1)OCCO2

Mol. weight [g/mol]: 178.18

CAS: 2879-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-118.33	kJ/mol	Joback Method
hf	-325.74	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hsub	102.50 ± 1.10	kJ/mol	NIST Webbook
hvap	57.61	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.660		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	588.29	K	Joback Method
tc	825.92	K	Joback Method
tf	375.65	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.86	J/mol×K	825.92	Joback Method

cpg	316.43	J/mol×K	588.29	Joback Method
cpg	329.57	J/mol×K	627.90	Joback Method
cpg	341.73	J/mol×K	667.50	Joback Method
cpg	352.99	J/mol×K	707.11	Joback Method
cpg	363.39	J/mol×K	746.71	Joback Method
cpg	372.99	J/mol×K	786.32	Joback Method
dvisc	0.0003887	Pa×s	588.29	Joback Method
dvisc	0.0022571	Pa×s	375.65	Joback Method
dvisc	0.0014837	Pa×s	411.09	Joback Method
dvisc	0.0010425	Pa×s	446.53	Joback Method
dvisc	0.0007715	Pa×s	481.97	Joback Method
dvisc	0.0005950	Pa×s	517.41	Joback Method
dvisc	0.0004744	Pa×s	552.85	Joback Method
hfust	23.49	kJ/mol	356.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2879201&Units=SI
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

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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation 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