

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	316.43	J/molxK	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
cpg	381.86	J/mol×K	825.92	Joback Method
dvisc	0.0022571	Paxs	375.65	Joback Method
dvisc	0.0014837	Paxs	411.09	Joback Method
dvisc	0.0010425	Paxs	446.53	Joback Method
dvisc	0.0007715	Paxs	481.97	Joback Method
dvisc	0.0005950	Paxs	517.41	Joback Method
dvisc	0.0004744	Paxs	552.85	Joback Method
dvisc	0.0003887	Paxs	588.29	Joback Method
hfust	23.49	kJ/mol	356.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2879201&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
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

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