5-Hydroxy-1-tetralone

Other names: 1(2H)-Naphthalenone, 3,4-dihydro-5-hydroxy-
1,2,3,4-tetrahydro-5-hydroxynaphthalen-1-one
5-Hydroxy-«alpha»-tetralone
5-Hydroxy-Â«alphaÂ»-tetralone
Inchi: InChI=1S/C10H10O2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1,3,5,11H,2,4,6H2
InchiKey: YPPZCRZRQHFRBH-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: O=C1CCCc2c(O)cccc21
Mol. weight [g/mol]: 162.19
CAS: 28315-93-7

Physical Properties

Property code	Value	Unit	Source
gf	-84.75	kJ/mol	Joback Method
hf	-252.70	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Energetics of Hydroxytetralones: A Calorimetric and Computational Thermochemical Study
hsub	118.50 ± 1.50	kJ/mol	NIST Webbook
hvap	58.45	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.911		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	623.98	K	Joback Method
tc	883.59	K	Joback Method
tf	440.00	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.64	J/mol×K	623.98	Joback Method

cpg	331.27	J/mol×K	667.25	Joback Method
cpg	343.88	J/mol×K	710.52	Joback Method
cpg	355.57	J/mol×K	753.79	Joback Method
cpg	366.46	J/mol×K	797.06	Joback Method
cpg	376.66	J/mol×K	840.33	Joback Method
cpg	386.27	J/mol×K	883.59	Joback Method
hfust	33.67	kJ/mol	480.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetics of Hydroxytetralones: A Calorimetric and Computational Thermochemical Study:	https://www.doi.org/10.1021/je8004408
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=C28315937&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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