

5-Methoxy-1-tetralone

Other names:	1(2H)-Naphthalenone, 3,4-dihydro-5-methoxy- 3,4-dihydro-5-methoxy-1(2H)-naphthalenone 5-methoxy-1,2,3,4-tetrahydronaphthalen-1-one «alpha»-Tetralone, 5-methoxy-
Inchi:	InChI=1S/C11H12O2/c1-13-11-7-3-4-8-9(11)5-2-6-10(8)12/h3-4,7H,2,5-6H2,1H3
InchiKey:	BRCPWISABURVIH-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	COc1cccc2c1CCCC2=O
Mol. weight [g/mol]:	176.21
CAS:	33892-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-36.34	kJ/mol	Joback Method
hf	-239.72	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hsub	97.90 ± 0.40	kJ/mol	NIST Webbook
hvap	50.73	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.214		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	593.64	K	Joback Method
tc	835.26	K	Joback Method
tf	374.30	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.14	J/mol×K	754.72	Joback Method
cpg	408.08	J/mol×K	794.99	Joback Method
cpg	338.90	J/mol×K	593.64	Joback Method
cpg	354.65	J/mol×K	633.91	Joback Method

cpg	369.43	J/mol×K	674.18	Joback Method
cpg	383.26	J/mol×K	714.45	Joback Method
cpg	419.09	J/mol×K	835.26	Joback Method
hfust	22.20	kJ/mol	362.50	NIST Webbook
hvapt	97.90	kJ/mol	298.15	Thermochemical study of some methoxytetralones

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	434.20	K	0.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33892750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study of some methoxytetralones:	https://www.doi.org/10.1016/j.jct.2008.07.021
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
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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