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]:	176.22

Physical Properties

Property code	Value	Unit	Source
hfus	13.17	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Cheméo Relay (1.0)
logp	2.214		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
tb	581.64	K	Cheméo Relay (1.0)
tf	359.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	396.14	J/mol×K	754.72	Joback Method
cpg	408.08	J/mol×K	794.99	Joback Method
cpg	419.09	J/mol×K	835.26	Joback Method
hvapt	97.90	kJ/mol	298.15	Thermochemical study of some methoxytetralones

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical study of some methoxytetralones:	https://www.doi.org/10.1016/j.jct.2008.07.021
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33892750&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point