

6-Methoxy-2-tetralone

Other names:	6-Methoxy-2-tetralone 6-methoxy-1,2,3,4-tetrahydronaphthalen-2-one
Inchi:	InChI=1S/C11H12O2/c1-13-11-5-3-8-6-10(12)4-2-9(8)7-11/h3,5,7H,2,4,6H2,1H3
InchiKey:	RMRKDYNVZWKAFP-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	COc1ccc2c(c1)CCC(=O)C2
Mol. weight [g/mol]:	176.22

Physical Properties

Property code	Value	Unit	Source
hfus	13.17	kJ/mol	Joback Method
logp	1.753		Crippen Method
mcvol	138.670	ml/mol	McGowan Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C247222&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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