

BENZOFURAN, 2,3-DIHYDRO-2,2,4,6-TETRAMETHYL-

Other names:	2,3-Dihydro-2,2,4,6-tetramethylbenzofuran
Inchi:	InChI=1S/C12H16O/c1-8-5-9(2)10-7-12(3,4)13-11(10)6-8/h5-6H,7H2,1-4H3
InchiKey:	NKEPZWFYNPDTND-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	<chem>Cc1cc(C)c2c(c1)OC(C)(C)C2</chem>
Mol. weight [g/mol]:	176.26

Physical Properties

Property code	Value	Unit	Source
hf	-170.76	kJ/mol	Cheméo Relay (1.0)
hfus	19.53	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Cheméo Relay (1.0)
logp	3.017		Crippen Method
mcvol	151.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.27	J/mol×K	549.51	Joback Method
cpg	379.11	J/mol×K	587.12	Joback Method
cpg	393.91	J/mol×K	624.73	Joback Method
cpg	407.82	J/mol×K	662.34	Joback Method
cpg	420.98	J/mol×K	699.95	Joback Method
cpg	433.55	J/mol×K	737.56	Joback Method
cpg	445.69	J/mol×K	775.17	Joback Method

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):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698495&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

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

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