

2,5-dimethyl-4-(3-methylbutoxy)-3(2H)furanone

Other names:	3(2H)-Furanone, 2,5-dimethyl-4-(3-methylbutoxy)
Inchi:	InChI=1S/C11H18O3/c1-7(2)5-6-13-11-9(4)14-8(3)10(11)12/h7-8H,5-6H2,1-4H3
InchiKey:	ATDNOZAARFGQGA-UHFFFAOYSA-N
Formula:	C11H18O3
SMILES:	CC1=C(OCCC(C)C)C(=O)C(C)O1
Mol. weight [g/mol]:	198.26

Physical Properties

Property code	Value	Unit	Source
hfus	23.78	kJ/mol	Joback Method
logp	2.268		Crippen Method
mcpvol	164.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.87	J/mol×K	592.23	Joback Method
cpg	443.30	J/mol×K	626.81	Joback Method
cpg	459.00	J/mol×K	661.38	Joback Method
cpg	473.94	J/mol×K	695.96	Joback Method
cpg	488.11	J/mol×K	730.54	Joback Method
cpg	501.50	J/mol×K	765.11	Joback Method
cpg	514.09	J/mol×K	799.69	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U322344&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

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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