3-Ketocarbofuran

Other names: Carbamic acid, methyl-, ester with 2,2-dimethyl-7-hydroxy-3(2H)-benzofuranone
3(2H)-Benzofuranone, 2,2-dimethyl-7-(((methylamino)carbonyl)oxy)-
3-Ketocarbofuran
Inchi: InChI=1S/C12H13NO4/c1-12(2)10(14)7-5-4-6-8(9(7)17-12)16-11(15)13-3/h4-6H,1-3H3,(
InchiKey: WXNZYYXXILQTKX-UHFFFAOYSA-N
Formula: C12H13NO4
SMILES: CNC(=O)Oc1cccc2c1OC(C)(C)C2=O
Mol. weight [g/mol]: 235.24

Physical Properties

Property code	Value	Unit	Source
hfus	27.31	kJ/mol	Joback Method
log10ws	-2.64		Cheméo Relay (1.0)
logp	1.758		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
tf	404.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.09	J/mol×K	738.81	Joback Method
cpg	493.79	J/mol×K	778.49	Joback Method
cpg	506.97	J/mol×K	818.17	Joback Method
cpg	519.73	J/mol×K	857.85	Joback Method
cpg	532.20	J/mol×K	897.53	Joback Method
cpg	544.50	J/mol×K	937.21	Joback Method
cpg	556.77	J/mol×K	976.89	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16709301&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point