Carbofuran 3-keto

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
CAS: 16709-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-154.67	kJ/mol	Joback Method
hf	-450.41	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	1.758		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	738.81	K	Joback Method
tc	976.89	K	Joback Method
tf	537.91	K	Joback Method
vc	0.641	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16709301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume