2-Cyclopenten-1-one, 5-butyl-3-methoxy-

Inchi: InChI=1S/C10H16O2/c1-3-4-5-8-6-9(12-2)7-10(8)11/h7-8H,3-6H2,1-2H3
InchiKey: CONTYKWBFDNXFF-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CCCCC1CC(OC)=CC1=O
Mol. weight [g/mol]: 168.23
CAS: 53690-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-137.39	kJ/mol	Joback Method
hf	-412.86	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.296		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	537.86	K	Joback Method
tc	744.83	K	Joback Method
tf	317.09	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.57	J/mol×K	537.86	Joback Method
cpg	362.58	J/mol×K	572.35	Joback Method
cpg	377.92	J/mol×K	606.85	Joback Method
cpg	392.57	J/mol×K	641.34	Joback Method
cpg	406.52	J/mol×K	675.84	Joback Method
cpg	419.77	J/mol×K	710.33	Joback Method
cpg	432.31	J/mol×K	744.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53690894&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume