3-Butyl-2-hydroxy-2-cyclopenten-1-one

Other names: 2-Cyclopenten-1-one, 3-butyl-2-hydroxy
Inchi: InChI=1S/C9H14O2/c1-2-3-4-7-5-6-8(10)9(7)11/h11H,2-6H2,1H3
InchiKey: UJTQSQADRGAFHN-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCCC1=C(O)C(=O)CC1
Mol. weight [g/mol]: 154.21
CAS: 29798-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-179.55	kJ/mol	Joback Method
hf	-403.36	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	58.74	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.352		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	594.39	K	Joback Method
tc	793.69	K	Joback Method
tf	361.17	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.33	J/mol×K	594.39	Joback Method
cpg	340.69	J/mol×K	627.61	Joback Method
cpg	352.48	J/mol×K	660.82	Joback Method
cpg	363.69	J/mol×K	694.04	Joback Method
cpg	374.34	J/mol×K	727.26	Joback Method
cpg	384.42	J/mol×K	760.47	Joback Method
cpg	393.94	J/mol×K	793.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29798729&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