2-butyl cyclopent-2-en-1 -one

Inchi: InChI=1S/C9H14O/c1-2-3-5-8-6-4-7-9(8)10/h6H,2-5,7H2,1H3
InchiKey: LQANWSYLRLMKDX-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CCCCC1=CCCC1=O
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-33.10	kJ/mol	Joback Method
hf	-239.66	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	41.39	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.466		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
ripol	1637.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	497.23	K	Joback Method
tc	709.66	K	Joback Method
tf	287.83	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.74	J/mol×K	497.23	Joback Method
cpg	289.69	J/mol×K	532.63	Joback Method
cpg	303.96	J/mol×K	568.04	Joback Method
cpg	317.53	J/mol×K	603.44	Joback Method
cpg	330.43	J/mol×K	638.85	Joback Method
cpg	342.66	J/mol×K	674.25	Joback Method
cpg	354.22	J/mol×K	709.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R319098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume