3-Phenylcyclobutenone

Inchi: InChI=1S/C10H8O/c11-10-6-9(7-10)8-4-2-1-3-5-8/h1-6H,7H2
InchiKey: IVOQFIKQFGCRBQ-UHFFFAOYSA-N
Formula: C10H8O
SMILES: O=C1C=C(c2ccccc2)C1
Mol. weight [g/mol]: 144.17
CAS: 38425-47-7

Physical Properties

Property code	Value	Unit	Source
chs	-5106.30 ± 1.20	kJ/mol	NIST Webbook
gf	99.83	kJ/mol	Joback Method
hf	-17.61	kJ/mol	Joback Method
hfs	27.80	kJ/mol	NIST Webbook
hfus	11.00	kJ/mol	Joback Method
hsub	58.60	kJ/mol	NIST Webbook
hvap	45.72	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.043		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	542.52	K	Joback Method
tc	794.75	K	Joback Method
tf	329.04	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.88	J/mol×K	542.52	Joback Method
cpg	264.03	J/mol×K	584.56	Joback Method
cpg	277.17	J/mol×K	626.60	Joback Method
cpg	289.34	J/mol×K	668.63	Joback Method
cpg	300.59	J/mol×K	710.67	Joback Method
cpg	310.95	J/mol×K	752.71	Joback Method

cpg	320.48	J/mol×K	794.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38425477&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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