2-Phenylglyoxylamide

Inchi: InChI=1S/C8H7NO2/c9-8(11)7(10)6-4-2-1-3-5-6/h1-5H,(H2,9,11)
InchiKey: WFRSBFQCMFWRTD-UHFFFAOYSA-N
Formula: C8H7NO2
SMILES: NC(=O)C(=O)c1ccccc1
Mol. weight [g/mol]: 149.15
CAS: 7505-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-62.50	kJ/mol	Joback Method
hf	-163.29	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.355		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	589.39	K	Joback Method
tc	830.19	K	Joback Method
tf	389.46	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.21	J/mol×K	589.39	Joback Method
cpg	265.57	J/mol×K	629.52	Joback Method
cpg	275.11	J/mol×K	669.66	Joback Method
cpg	283.86	J/mol×K	709.79	Joback Method
cpg	291.88	J/mol×K	749.93	Joback Method
cpg	299.19	J/mol×K	790.06	Joback Method
cpg	305.84	J/mol×K	830.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7505922&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

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