2H-1,4-Benzoxazin-3(4H)-one

Other names: 2H-1,4-Benzoxazin-3-one
3-Keto-4-aza-2,3-dihydrobenzopyran
Inchi: InChI=1S/C8H7NO2/c10-8-5-11-7-4-2-1-3-6(7)9-8/h1-4H,5H2,(H,9,10)
InchiKey: QRCGFTXRXYMJOS-UHFFFAOYSA-N
Formula: C8H7NO2
SMILES: OC1=Nc2ccccc2OC1
Mol. weight [g/mol]: 149.15
CAS: 5466-88-6

Physical Properties

Property code	Value	Unit	Source
gf	89.79	kJ/mol	Joback Method
hf	-63.36	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hsub	106.40 ± 3.00	kJ/mol	NIST Webbook
hvap	65.09	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.667		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	5273.90	kPa	Joback Method
tb	606.75	K	Joback Method
tc	837.88	K	Joback Method
tf	409.73	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.68	J/mol×K	606.75	Joback Method
cpg	278.39	J/mol×K	645.27	Joback Method
cpg	288.29	J/mol×K	683.79	Joback Method
cpg	297.43	J/mol×K	722.32	Joback Method
cpg	305.84	J/mol×K	760.84	Joback Method
cpg	313.55	J/mol×K	799.36	Joback Method

cpg	320.61	J/mol×K	837.88	Joback Method
hfust	22.80	kJ/mol	445.60	NIST Webbook

Sources

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=C5466886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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