4-oxo-3,4-dihydro-2,3-diazaphenoxathiin

Inchi: InChI=1S/C10H8N2O2S/c13-10-9-8(5-11-12-10)15-7-4-2-1-3-6(7)14-9/h1-5,8-9H,(H,12,1
InchiKey: XHWIEBKKBFMEQX-UHFFFAOYSA-N
Formula: C10H8N2O2S
SMILES: O=C1NN=CC2Sc3ccccc3OC12
Mol. weight [g/mol]: 220.25

Physical Properties

Property code	Value	Unit	Source
gf	299.00	kJ/mol	Joback Method
hf	50.73	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.024		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
rinpol	1775.00		NIST Webbook
tb	725.89	K	Joback Method
tc	1022.46	K	Joback Method
tf	625.81	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.73	J/mol×K	725.89	Joback Method
cpg	426.24	J/mol×K	775.32	Joback Method
cpg	440.09	J/mol×K	824.75	Joback Method
cpg	452.30	J/mol×K	874.18	Joback Method
cpg	462.91	J/mol×K	923.61	Joback Method
cpg	471.96	J/mol×K	973.03	Joback Method
cpg	479.48	J/mol×K	1022.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496269&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume