2-Phenylbenzoxazone-4

Inchi: InChI=1S/C14H11NO2/c16-13-11-8-4-5-9-12(11)17-14(15-13)10-6-2-1-3-7-10/h1-9,14H,(

InchiKey: AMZRLVJMBHMIPA-UHFFFAOYSA-N

Formula: C14H11NO2

SMILES: O=C1NC(c2ccccc2)Oc2ccccc21

Mol. weight [g/mol]: 225.24

CAS: 6629-80-7

Physical Properties

Property code	Value	Unit	Source
gf	209.84	kJ/mol	Joback Method
hf	-35.95	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.508		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	732.39	K	Joback Method
tc	1009.69	K	Joback Method
tf	527.14	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.07	J/mol×K	732.39	Joback Method
cpg	476.20	J/mol×K	778.61	Joback Method
cpg	490.77	J/mol×K	824.82	Joback Method
cpg	503.84	J/mol×K	871.04	Joback Method
cpg	515.48	J/mol×K	917.26	Joback Method
cpg	525.74	J/mol×K	963.47	Joback Method
cpg	534.67	J/mol×K	1009.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6629807&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