

3-Phenyloxindole

Inchi:	InChI=1S/C14H11NO/c16-14-13(10-6-2-1-3-7-10)11-8-4-5-9-12(11)15-14/h1-9,13H,(H,15)
InchiKey:	PAMMIXSSIGTOAK-UHFFFAOYSA-N
Formula:	C14H11NO
SMILES:	O=C1Nc2ccccc2C1c1ccccc1
Mol. weight [g/mol]:	209.24
CAS:	3456-79-9

Physical Properties

Property code	Value	Unit	Source
gf	308.06	kJ/mol	Joback Method
hf	102.21	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.771		Crippen Method
mvol	161.290	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	701.17	K	Joback Method
tc	974.74	K	Joback Method
tf	504.09	K	Joback Method
vc	0.605	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.57	J/mol×K	701.17	Joback Method
cpg	444.91	J/mol×K	746.77	Joback Method
cpg	459.82	J/mol×K	792.36	Joback Method
cpg	473.36	J/mol×K	837.96	Joback Method
cpg	485.62	J/mol×K	883.55	Joback Method
cpg	496.66	J/mol×K	929.15	Joback Method
cpg	506.57	J/mol×K	974.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3456799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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