

1-Benzoxepin-5-carboxylic acid,2,3,4,5-tetrahydro-3-hydroxy-5-phenyl-,gamma

Inchi:	InChI=1S/C17H14O3/c18-16-17(12-6-2-1-3-7-12)10-13(20-16)11-19-15-9-5-4-8-14(15)17
InchiKey:	MBKUQWVLMRJNIJ-UHFFFAOYSA-N
Formula:	C17H14O3
SMILES:	O=C1OC2COc3ccccc3C1(c1cccc1)C2
Mol. weight [g/mol]:	266.29
CAS:	94540-95-1

Physical Properties

Property code	Value	Unit	Source
gf	116.53	kJ/mol	Joback Method
hf	-179.64	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.681		Crippen Method
mcvol	194.460	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	786.41	K	Joback Method
tc	1066.14	K	Joback Method
tf	524.33	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.72	J/molxK	786.41	Joback Method
cpg	601.82	J/molxK	833.03	Joback Method
cpg	619.19	J/molxK	879.65	Joback Method
cpg	636.17	J/molxK	926.28	Joback Method
cpg	653.10	J/molxK	972.90	Joback Method
cpg	670.30	J/molxK	1019.52	Joback Method
cpg	688.12	J/molxK	1066.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94540951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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