Isoquinoline, 1-benzyl-1,2,3,4-tetrahydro-

Inchi: InChI=1S/C16H17N/c1-2-6-13(7-3-1)12-16-15-9-5-4-8-14(15)10-11-17-16/h1-9,16-17H,1
InchiKey: YRYCIFUZSUMAAY-UHFFFAOYSA-N
Formula: C16H17N
SMILES: c1ccc(CC2NCCc3ccccc32)cc1
Mol. weight [g/mol]: 223.31
CAS: 19716-56-4

Physical Properties

Property code	Value	Unit	Source
gf	435.39	kJ/mol	Joback Method
hf	192.47	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.116		Crippen Method
mcvol	187.900	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	683.38	K	Joback Method
tc	941.58	K	Joback Method
tf	454.89	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.73	J/mol×K	683.38	Joback Method
cpg	527.03	J/mol×K	726.41	Joback Method
cpg	544.74	J/mol×K	769.45	Joback Method
cpg	560.97	J/mol×K	812.48	Joback Method
cpg	575.86	J/mol×K	855.51	Joback Method
cpg	589.50	J/mol×K	898.54	Joback Method
cpg	602.02	J/mol×K	941.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19716564&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