3-BENZYLQUINOLINE

Inchi: InChI=1S/C16H13N/c1-2-6-13(7-3-1)10-14-11-15-8-4-5-9-16(15)17-12-14/h1-9,11-12H,1
InchiKey: QVMSGEZMPYTLKN-UHFFFAOYSA-N
Formula: C16H13N
SMILES: c1ccc(Cc2cnc3ccccc3c2)cc1
Mol. weight [g/mol]: 219.29

Physical Properties

Property code	Value	Unit	Source
af	0.5151		Cheméo Relay (1.0)
hf	309.04	kJ/mol	Cheméo Relay (1.0)
hvap	95.85	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-3.95		Cheméo Relay (1.0)
logp	3.826		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
pc	3251.21	kPa	Cheméo Relay (1.0, beta)
tb	652.30	K	Cheméo Relay (1.0)
tc	927.75	K	Cheméo Relay (1.0)
tf	339.00 ± 1.00	K	NIST Webbook
vc	0.676	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.00	K	2.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37045162&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume