2-BENZYLQUINOLINE

Inchi: InChI=1S/C16H13N/c1-2-6-13(7-3-1)12-15-11-10-14-8-4-5-9-16(14)17-15/h1-11H,12H2
InchiKey: LLVHFJHCODIQJH-UHFFFAOYSA-N
Formula: C16H13N
SMILES: c1ccc(Cc2ccc3ccccc3n2)cc1
Mol. weight [g/mol]: 219.29

Physical Properties

Property code	Value	Unit	Source
af	0.5060		Cheméo Relay (1.0)
hf	301.55	kJ/mol	Cheméo Relay (1.0)
hvap	95.03	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	3.826		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
pc	3206.77	kPa	Cheméo Relay (1.0, beta)
tb	636.68	K	Cheméo Relay (1.0)
tc	919.49	K	Cheméo Relay (1.0)
tf	346.59	K	Cheméo Relay (1.0)
vc	0.679	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.50 ± 2.50	K	0.01	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1745773&Units=SI

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