6-BENZYLQUINOLINE

Other names: Quinoline, 6-(phenylmethyl)-
Inchi: InChI=1S/C16H13N/c1-2-5-13(6-3-1)11-14-8-9-16-15(12-14)7-4-10-17-16/h1-10,12H,11H
InchiKey: GMGJJCVVIGBOAJ-UHFFFAOYSA-N
Formula: C16H13N
SMILES: c1ccc(Cc2ccc3ncccc3c2)cc1
Mol. weight [g/mol]: 219.29

Physical Properties

Property code	Value	Unit	Source
af	0.5162		Cheméo Relay (1.0)
hf	295.69	kJ/mol	Cheméo Relay (1.0)
hvap	97.62	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-3.85		Cheméo Relay (1.0)
logp	3.826		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
pc	3285.00	kPa	Cheméo Relay (1.0, beta)
tb	653.17	K	Cheméo Relay (1.0)
tc	923.59	K	Cheméo Relay (1.0)
tf	352.50 ± 0.50	K	NIST Webbook
vc	0.675	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.70	K	0.10	NIST Webbook
tbrp	413.50 ± 1.50	K	0.10	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54884990&Units=SI
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

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