6-METHOXYQUINOLINE

Other names:	6-Methoxyquinoline
	p-Quinanisole
	methyl 6-quinolyl ether
Inchi:	InChI=1S/C10H9NO/c1-12-9-4-5-10-8(7-9)3-2-6-11-10/h2-7H,1H3
InchiKey:	HFDLDPJYCIEXJP-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	COc1ccc2ncccc2c1
Mol. weight [g/mol]:	159.19

Physical Properties

Property code	Value	Unit	Source
af	0.4721		Cheméo Relay (1.0)
hf	57.36	kJ/mol	Cheméo Relay (1.0)
hvap	78.10 ± 2.30	kJ/mol	NIST Webbook
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-2.16		Cheméo Relay (1.0)
logp	2.243		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
pc	4162.92	kPa	Cheméo Relay (1.0, beta)
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
ripol	2353.00		NIST Webbook
tb	559.81	K	Cheméo Relay (1.0)
tc	809.22	K	Cheméo Relay (1.0)
tf	313.80	K	Cheméo Relay (1.0)
vc	0.464	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	466.20	K	6.70	NIST Webbook
tbrp	426.20	K	1.60	NIST Webbook
tbrp	416.00 ± 3.00	K	2.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5263876&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
Cheméo Relay (1.0):	

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume