

6-methyloisoquinoline

Inchi:	InChI=1S/C10H9N/c1-8-2-3-10-7-11-5-4-9(10)6-8/h2-7H,1H3
InchiKey:	PPEJLOXOMBAXES-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1ccc2cnccc2c1
Mol. weight [g/mol]:	143.19
CAS:	42398-73-2

Physical Properties

Property code	Value	Unit	Source
af	0.4016		Cheméo Relay (1.0)
gf	249.99	kJ/mol	Cheméo Relay (1.0, beta)
hf	177.03	kJ/mol	Cheméo Relay (1.0)
hvap	64.90	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-2.02		Cheméo Relay (1.0)
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4481.05	kPa	Cheméo Relay (1.0, beta)
tb	541.22	K	Cheméo Relay (1.0)
tc	804.58	K	Cheméo Relay (1.0)
tf	335.04	K	Cheméo Relay (1.0)
vc	0.442	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54978e+01
Coeff. B	-4.66231e+03
Coeff. C	-9.08950e+01
Temperature range (K), min.	358.65
Temperature range (K), max.	548.60

Sources

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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