Quinoline, 2,6-dimethyl-

Other names:	2,6-Dimethylquinoline
	6-METHYLQUINALDINE
	P-TOLUQUINALDINE
	quinaldine, 6-methyl-
Inchi:	InChI=1S/C11H11N/c1-8-3-6-11-10(7-8)5-4-9(2)12-11/h3-7H,1-2H3
InchiKey:	JJPSZKIOGBRMHK-UHFFFAOYSA-N
Formula:	C11H11N
SMILES:	Cc1ccc2nc(C)ccc2c1
Mol. weight [g/mol]:	157.21
CAS:	877-43-0

Physical Properties

Property code	Value	Unit	Source
af	0.3700		KDB
chs	-5937.10 ± 2.00	kJ/mol	NIST Webbook
hf	120.90 ± 2.90	kJ/mol	NIST Webbook
hfs	36.40 ± 2.90	kJ/mol	NIST Webbook
hfus	20.42	kJ/mol	Thermodynamic properties of methylquinolines: Experimental results for 2,6-dimethylquinoline and mutual validation between experiments and computational methods for methylquinolines
hsub	84.50 ± 1.50	kJ/mol	NIST Webbook
hsub	84.50 ± 1.50	kJ/mol	NIST Webbook
hsub	84.50	kJ/mol	NIST Webbook
hvap	67.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.99		Crippen Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
pc	3900.00	kPa	KDB
rinpol	1397.00		NIST Webbook
rinpol	243.76		NIST Webbook
rinpol	244.19		NIST Webbook
rinpol	242.43		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1397.00		NIST Webbook

rinpol	1414.00		NIST Webbook
rinpol	243.76		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1397.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2044.00		NIST Webbook
tb	539.15 ± 1.00	K	NIST Webbook
tb	538.55 ± 0.06	K	NIST Webbook
tb	539.70	K	NIST Webbook
tb	538.60	K	KDB
tc	804.00	K	KDB
tf	288.00	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.40	kJ/mol	330.80	NIST Webbook
hvapt	64.00 ± 0.10	kJ/mol	464.00	NIST Webbook
hvapt	61.10 ± 0.10	kJ/mol	464.00	NIST Webbook
hvapt	55.70 ± 0.10	kJ/mol	464.00	NIST Webbook
hvapt	53.00 ± 0.10	kJ/mol	464.00	NIST Webbook
hvapt	50.00 ± 0.20	kJ/mol	464.00	NIST Webbook
hvapt	46.80 ± 0.40	kJ/mol	464.00	NIST Webbook
hvapt	55.70	kJ/mol	501.00	NIST Webbook
hvapt	58.40 ± 0.10	kJ/mol	464.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39422e+01
Coeff. B	-4.18485e+03

Coeff. C	-9.08700e+01
Temperature range (K), min.	397.35
Temperature range (K), max.	575.75

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of methylquinolines: Experimental results for 2,6-dimethylquinoline and mutual validation between experiments and computational methods for methylquinolines:	https://www.doi.org/10.1016/j.jct.2006.10.012
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1372.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C877430&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point