Quinoline, 8-methyl-

Other names: 8-Methylquinoline
Inchi: InChI=1S/C10H9N/c1-8-4-2-5-9-6-3-7-11-10(8)9/h2-7H,1H3
InchiKey: JRLTTZUODKEYDH-UHFFFAOYSA-N
Formula: C10H9N
SMILES: Cc1cccc2cccnc12
Mol. weight [g/mol]: 143.19
CAS: 611-32-5

Physical Properties

Property code	Value	Unit	Source
af	0.3910		KDB
chl	-5323.30 ± 2.00	kJ/mol	NIST Webbook
hf	167.70 ± 3.10	kJ/mol	NIST Webbook
hfl	102.00 ± 2.40	kJ/mol	NIST Webbook
hfus	10.73	kJ/mol	The thermodynamic properties of 2-methylquinoline and 8 methylquinoline
hvap	65.70 ± 1.90	kJ/mol	NIST Webbook
hvap	65.70	kJ/mol	NIST Webbook
hvap	65.70 ± 1.90	kJ/mol	NIST Webbook
hvap	62.10 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	5000.00	kPa	KDB
rinpol	1304.00		NIST Webbook
rinpol	1304.50		NIST Webbook
rinpol	1313.90		NIST Webbook
rinpol	1289.50		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	225.39		NIST Webbook
rinpol	225.18		NIST Webbook
rinpol	223.02		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1304.00		NIST Webbook

rinpol	1313.90		NIST Webbook
rinpol	1304.50		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1319.50		NIST Webbook
rinpol	1319.50		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1929.00		NIST Webbook
ripol	1929.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	520.90	K	KDB
tb	519.00 ± 2.00	K	NIST Webbook
tb	521.10 ± 0.30	K	NIST Webbook
tb	520.70	K	NIST Webbook
tb	521.05 ± 0.15	K	NIST Webbook
tb	521.15 ± 0.70	K	NIST Webbook
tc	791.00	K	KDB
tf	246.50 ± 0.20	K	NIST Webbook
tf	193.00	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	10.73	kJ/mol	246.90	NIST Webbook
hvapt	59.20 ± 0.10	kJ/mol	438.50	NIST Webbook
hvapt	56.60 ± 0.10	kJ/mol	438.50	NIST Webbook
hvapt	54.00 ± 0.10	kJ/mol	438.50	NIST Webbook
hvapt	51.30 ± 0.10	kJ/mol	438.50	NIST Webbook
hvapt	49.00 ± 0.20	kJ/mol	438.50	NIST Webbook
hvapt	46.20 ± 0.30	kJ/mol	438.50	NIST Webbook
hvapt	52.20	kJ/mol	508.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	4.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39943e+01
Coeff. B	-4.07568e+03
Coeff. C	-8.60070e+01
Temperature range (K), min.	383.36
Temperature range (K), max.	555.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.80987e+01
Coeff. B	-8.16507e+03
Coeff. C	-4.51250e+00
Coeff. D	1.53970e-06
Temperature range (K), min.	493.15
Temperature range (K), max.	523.15

Sources

The thermodynamic properties of 2-methylquinoline and 8 methylquinoline:	https://www.doi.org/10.1021/je049595u
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1370.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611325&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1370
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
chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point