N-Methyl-p-cumidine

Other names: Aniline, p-isopropyl-N-methyl-,
Inchi: InChI=1S/C10H15N/c1-8(2)9-4-6-10(11-3)7-5-9/h4-8,11H,1-3H3
InchiKey: RQZGOIJRSJWNRB-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CNc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 149.23
CAS: 6950-79-4

Physical Properties

Property code	Value	Unit	Source
gf	223.05	kJ/mol	Joback Method
hf	23.52	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.852		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1286.40		NIST Webbook
tb	509.59	K	Joback Method
tc	721.82	K	Joback Method
tf	279.06	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.12	J/mol×K	509.59	Joback Method
cpg	320.37	J/mol×K	544.96	Joback Method
cpg	334.75	J/mol×K	580.33	Joback Method
cpg	348.31	J/mol×K	615.70	Joback Method
cpg	361.08	J/mol×K	651.07	Joback Method
cpg	373.08	J/mol×K	686.44	Joback Method
cpg	384.35	J/mol×K	721.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39528e+01
Coeff. B	-4.04365e+03
Coeff. C	-8.07150e+01
Temperature range (K), min.	376.62
Temperature range (K), max.	548.66

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6950794&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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