

4-isobutylaniline

Inchi:	InChI=1S/C10H15N/c1-8(2)7-9-3-5-10(11)6-4-9/h3-6,8H,7,11H2,1-2H3
InchiKey:	JSHQATXVCGCYJQ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)Cc1ccc(N)cc1
Mol. weight [g/mol]:	149.24
CAS:	30090-17-6

Physical Properties

Property code	Value	Unit	Source
af	0.5369		Cheméo Relay (1.0)
hf	-30.33	kJ/mol	Cheméo Relay (1.0)
hfus	16.98	kJ/mol	Joback Method
hvap	65.31	kJ/mol	Cheméo Relay (1.0)
ie	7.63	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	2.467		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	519.61	K	Cheméo Relay (1.0)
tc	730.68	K	Cheméo Relay (1.0)
tf	281.77	K	Cheméo Relay (1.0)
vc	0.489	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.49	J/mol×K	531.95	Joback Method
cpg	331.53	J/mol×K	568.92	Joback Method
cpg	345.68	J/mol×K	605.89	Joback Method
cpg	358.96	J/mol×K	642.86	Joback Method
cpg	371.42	J/mol×K	679.83	Joback Method
cpg	383.09	J/mol×K	716.80	Joback Method
cpg	394.01	J/mol×K	753.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45567e+01
Coeff. B	-4.28283e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	383.12
Temperature range (K), max.	546.22

Sources

The Yaws Handbook of Vapor Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
https://en.wikipedia.org/wiki/Joback_method

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):

Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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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