4-Isopropylbenzonitrile

Other names:	4-(1-Methylethyl)benzonitrile
	Benzonitrile, p-isopropyl-
	Cuminyl nitrile
	p-Cyanocumene
	p-Isopropylbenzonitrile
Inchi:	InChI=1S/C10H11N/c1-8(2)10-5-3-9(7-11)4-6-10/h3-6,8H,1-2H3
InchiKey:	YFDJCWXBKWRDPW-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	CC(C)c1ccc(C#N)cc1
Mol. weight [g/mol]:	145.21
CAS:	13816-33-6

Physical Properties

Property code	Value	Unit	Source
af	0.4270		Cheméo Relay (1.0)
gf	266.84	kJ/mol	Joback Method
hf	114.91	kJ/mol	Cheméo Relay (1.0)
hfus	13.29	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-3.45		Cheméo Relay (1.0)
logp	2.682		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	510.74	K	Cheméo Relay (1.0)
tc	735.32	K	Cheméo Relay (1.0)
tf	273.15	K	Cheméo Relay (1.0)
vc	0.464	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.12	J/mol×K	561.50	Joback Method
cpg	300.69	J/mol×K	599.73	Joback Method

cpg	312.46	J/mol×K	637.97	Joback Method
cpg	323.47	J/mol×K	676.20	Joback Method
cpg	333.74	J/mol×K	714.44	Joback Method
cpg	343.31	J/mol×K	752.67	Joback Method
cpg	352.22	J/mol×K	790.91	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.85669e+01
Coeff. B	-5.96761e+03
Coeff. C	-9.96520e+01
Temperature range (K), min.	426.12
Temperature range (K), max.	549.85

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13816336&Units=SI

Joback Method: 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

Legend

af: Acentric Factor

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
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