Benzonitrile, 4-(1-methylethyl)-

Other names:	4-(1-Methylethyl)benzonitrile
	4-Isopropylbenzonitrile
	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]:	145.20
CAS:	13816-33-6

Physical Properties

Property code	Value	Unit	Source
gf	266.84	kJ/mol	Joback Method
hf	134.93	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.682		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	561.50	K	Joback Method
tc	790.91	K	Joback Method
tf	291.39	K	Joback Method
vc	0.507	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13816336&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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