4-Butylbenzonitrile

Other names: 1-Butyl-4-cyanobenzene
Benzonitrile,4-butyl-
Inchi: InChI=1S/C11H13N/c1-2-3-4-10-5-7-11(9-12)8-6-10/h5-8H,2-4H2,1H3
InchiKey: KGZNJCXNPLUEQS-UHFFFAOYSA-N
Formula: C11H13N
SMILES: CCCCc1ccc(C#N)cc1
Mol. weight [g/mol]: 159.23
CAS: 20651-73-4

Physical Properties

Property code	Value	Unit	Source
gf	277.70	kJ/mol	Joback Method
hf	119.57	kJ/mol	Joback Method
hfus	19.40	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
ie	10.10 ± 0.10	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	2.901		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	584.82	K	Joback Method
tc	805.11	K	Joback Method
tf	317.66	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.73	J/mol×K	584.82	Joback Method
cpg	346.84	J/mol×K	621.53	Joback Method
cpg	359.15	J/mol×K	658.25	Joback Method
cpg	370.71	J/mol×K	694.96	Joback Method
cpg	381.54	J/mol×K	731.68	Joback Method
cpg	391.67	J/mol×K	768.39	Joback Method

cpg	401.14	J/mol×K	805.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34482e+01
Coeff. B	-4.04701e+03
Coeff. C	-8.95550e+01
Temperature range (K), min.	397.07
Temperature range (K), max.	586.93

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20651734&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

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