Benzenebutanenitrile

Other names:	Butyronitrile, 4-phenyl- 4-Phenylbutyronitrile «gamma»-Phenylpropyl cyanide (3-Cyanopropyl)benzene 1-Cyano-3-phenylpropane 4-Phenylbutanenitrile NSC 1853 Gamma-phenylbutyronitrile
Inchi:	InChI=1S/C10H11N/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8H2
InchiKey:	ICMVGKQFVMTRLB-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	N#CCCCc1ccccc1
Mol. weight [g/mol]:	145.20
CAS:	2046-18-6

Physical Properties

Property code	Value	Unit	Source
gf	278.91	kJ/mol	Joback Method
hf	151.68	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.533		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1336.70		NIST Webbook
tb	556.96	K	Joback Method
tc	780.24	K	Joback Method
tf	293.87	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	288.38	J/mol×K	556.96	Joback Method
cpg	300.91	J/mol×K	594.17	Joback Method
cpg	312.64	J/mol×K	631.39	Joback Method
cpg	323.58	J/mol×K	668.60	Joback Method
cpg	333.80	J/mol×K	705.81	Joback Method
cpg	343.31	J/mol×K	743.03	Joback Method
cpg	352.17	J/mol×K	780.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	0.30	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2046186&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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