

Butanenitrile, 2-phenyl

Other names:	DL-2-phenylbutyronitrile Benzeneacetonitrile, «alpha»-ethyl-
Inchi:	InChI=1S/C10H11N/c1-2-9(8-11)10-6-4-3-5-7-10/h3-7,9H,2H2,1H3
InchiKey:	IZPUPXNVRNBDSW-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	CCC(C#N)c1ccccc1
Mol. weight [g/mol]:	145.20
CAS:	769-68-6

Physical Properties

Property code	Value	Unit	Source
gf	276.47	kJ/mol	Joback Method
hf	146.40	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	64.30 ± 0.60	kJ/mol	NIST Webbook
log10ws	-2.94		Crippen Method
logp	2.704		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1304.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2129.00		NIST Webbook
tb	556.52	K	Joback Method
tc	784.84	K	Joback Method
tf	278.87	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/mol×K	556.52	Joback Method
cpg	301.64	J/mol×K	594.57	Joback Method
cpg	313.67	J/mol×K	632.63	Joback Method
cpg	324.87	J/mol×K	670.68	Joback Method

cpg	335.30	J/mol×K	708.73	Joback Method
cpg	344.98	J/mol×K	746.78	Joback Method
cpg	353.97	J/mol×K	784.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	2.00	NIST Webbook

Sources

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=C769686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	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

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