

1-PHENYL-1-CYCLOPROPANECARBONITRILE

Other names:	Cyclopropanecarbonitrile, 1-phenyl- 1-Phenyl-cyclopropanecarbonitrile
Inchi:	InChI=1S/C10H9N/c11-8-10(6-7-10)9-4-2-1-3-5-9/h1-5H,6-7H2
InchiKey:	ZHFURHRJUWYDKG-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	N#CC1(c2ccccc2)CC1
Mol. weight [g/mol]:	143.19

Physical Properties

Property code	Value	Unit	Source
hf	308.70	kJ/mol	Cheméo Relay (1.0)
hfus	9.04	kJ/mol	Joback Method
ie	8.86	eV	Cheméo Relay (1.0)
logp	2.242		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
tf	357.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.11	J/mol×K	563.94	Joback Method
cpg	284.73	J/mol×K	605.79	Joback Method
cpg	296.22	J/mol×K	647.64	Joback Method
cpg	306.83	J/mol×K	689.49	Joback Method
cpg	316.77	J/mol×K	731.34	Joback Method
cpg	326.28	J/mol×K	773.19	Joback Method
cpg	335.59	J/mol×K	815.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C935444&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/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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