1-BENZOCYCLOBUTENECARBONITRILE

Inchi: InChI=1S/C9H7N/c10-6-8-5-7-3-1-2-4-9(7)8/h1-4,8H,5H2
InchiKey: FJIDKRPZJBUHME-UHFFFAOYSA-N
Formula: C9H7N
SMILES: N#CC1Cc2ccccc21
Mol. weight [g/mol]: 129.16

Physical Properties

Property code	Value	Unit	Source
hfus	14.46	kJ/mol	Joback Method
logp	1.850		Crippen Method
mcvol	104.430	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.37	J/mol×K	541.53	Joback Method
cpg	239.31	J/mol×K	581.18	Joback Method
cpg	249.36	J/mol×K	620.82	Joback Method
cpg	258.61	J/mol×K	660.47	Joback Method
cpg	267.12	J/mol×K	700.12	Joback Method
cpg	275.00	J/mol×K	739.76	Joback Method
cpg	282.31	J/mol×K	779.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.50 ± 1.50	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6809912&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure