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
CAS: 6809-91-2

Physical Properties

Property code	Value	Unit	Source
gf	333.71	kJ/mol	Joback Method
hf	239.81	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.850		Crippen Method
mcvol	104.430	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	541.53	K	Joback Method
tc	779.41	K	Joback Method
tf	316.58	K	Joback Method
vc	0.422	m3/kmol	Joback 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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6809912&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume