Bicyclo[2.2.1]hexa-2,5-diene, 2,3-dicarbonitrile-

Other names: 2,3-Dicyanobicyclo[2.2.1]hepta-2,5-diene
Norbornadiene-2,3-dicarbonitrile

Inchi: InChI=1S/C9H6N2/c10-4-8-6-1-2-7(3-6)9(8)5-11/h1-2,6-7H,3H2

InchiKey: XKDBHCJBKRLHRJ-UHFFFAOYSA-N

Formula: C9H6N2

SMILES: N#CC1=C(C#N)C2C=CC1C2

Mol. weight [g/mol]: 142.16

CAS: 825-24-1

Physical Properties

Property code	Value	Unit	Source
gf	441.32	kJ/mol	Joback Method
hf	332.73	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-2.34		Crippen Method
logp	1.536		Crippen Method
mcvol	110.110	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	635.51	K	Joback Method
tc	877.23	K	Joback Method
tf	380.09	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.33	J/mol×K	635.51	Joback Method
cpg	274.36	J/mol×K	675.80	Joback Method
cpg	282.72	J/mol×K	716.08	Joback Method

cpg	290.46	J/mol×K	756.37	Joback Method
cpg	297.69	J/mol×K	796.66	Joback Method
cpg	304.48	J/mol×K	836.94	Joback Method
cpg	310.91	J/mol×K	877.23	Joback Method

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=C825241&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
ie: Ionization energy
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume