Bicyclo[2.2.2]oct-5-ene-2,2,3,3-tetracarbonitrile

Inchi: InChI=1S/C12H8N4/c13-5-11(6-14)9-1-2-10(4-3-9)12(11,7-15)8-16/h1-2,9-10H,3-4H2
InchiKey: GFDRDNGZQZLSRI-UHFFFAOYSA-N
Formula: C12H8N4
SMILES: N#CC1(C#N)C2C=CC(CC2)C1(C#N)C#N
Mol. weight [g/mol]: 208.22
CAS: 1017-93-2

Physical Properties

Property code	Value	Unit	Source
gf	683.74	kJ/mol	Joback Method
hf	687.40	kJ/mol	NIST Webbook
hfus	15.70	kJ/mol	Joback Method
hsub	112.00 ± 5.40	kJ/mol	NIST Webbook
hvap	81.76	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	1.650		Crippen Method
mcvol	159.440	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	894.60	K	Joback Method
tc	1160.88	K	Joback Method
tf	553.88	K	Joback Method
tt	533.20 ± 2.00	K	NIST Webbook
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.34	J/mol×K	894.60	Joback Method
cpg	480.45	J/mol×K	938.98	Joback Method
cpg	497.24	J/mol×K	983.36	Joback Method
cpg	516.13	J/mol×K	1027.74	Joback Method
cpg	537.53	J/mol×K	1072.12	Joback Method
cpg	561.86	J/mol×K	1116.50	Joback Method
cpg	589.54	J/mol×K	1160.88	Joback Method

hfust	4.54	kJ/mol	533.20	NIST Webbook
hsubt	111.70 ± 5.40	kJ/mol	433.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1017932&Units=SI
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

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume