Benzene-1,2,4-tricarbonitrile

Inchi: InChI=1S/C9H3N3/c10-4-7-1-2-8(5-11)9(3-7)6-12/h1-3H
InchiKey: RTJRHFSBKHHQEI-UHFFFAOYSA-N
Formula: C9H3N3
SMILES: N#Cc1ccc(C#N)c(C#N)c1
Mol. weight [g/mol]: 153.14
CAS: 10347-14-5

Physical Properties

Property code	Value	Unit	Source
gf	517.59	kJ/mol	Joback Method
hf	479.14	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.302		Crippen Method
mcvol	118.050	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	748.20	K	Joback Method
tc	1003.02	K	Joback Method
tf	437.62	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.51	J/mol×K	748.20	Joback Method
cpg	265.61	J/mol×K	790.67	Joback Method
cpg	271.18	J/mol×K	833.14	Joback Method
cpg	276.25	J/mol×K	875.61	Joback Method
cpg	280.86	J/mol×K	918.08	Joback Method
cpg	285.01	J/mol×K	960.55	Joback Method
cpg	288.73	J/mol×K	1003.02	Joback Method

Sources

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=C10347145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume