Isocyanobenzene-2,4,6-d3

Inchi: InChI=1S/C7H5N/c1-8-7-5-3-2-4-6-7/h2-6H/i2D,5D,6D
InchiKey: RCIBIGQXGCBBCT-UJESMPABSA-N
Formula: C7H2D3N
SMILES: [C-]#[N+]c1ccccc1
Mol. weight [g/mol]: 106.14
CAS: 51524-87-9

Physical Properties

Property code	Value	Unit	Source
gf	253.65	kJ/mol	Joback Method
hf	213.60	kJ/mol	Joback Method
hfus	9.43	kJ/mol	Joback Method
hvap	43.93	kJ/mol	Joback Method
ie	9.90 ± 0.20	eV	NIST Webbook
log10ws	-4.22		Crippen Method
logp	2.237		Crippen Method
mcvol	87.110	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	488.32	K	Joback Method
tc	724.27	K	Joback Method
tf	260.06	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.30	J/mol×K	488.32	Joback Method
cpg	170.44	J/mol×K	527.64	Joback Method
cpg	178.93	J/mol×K	566.97	Joback Method
cpg	186.79	J/mol×K	606.29	Joback Method
cpg	194.06	J/mol×K	645.62	Joback Method
cpg	200.77	J/mol×K	684.94	Joback Method
cpg	206.96	J/mol×K	724.27	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=C51524879&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
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