3-(CH3)2NC6H4CN

Inchi: InChI=1S/C9H10N2/c1-11(2)9-5-3-4-8(6-9)7-10/h3-6H,1-2H3
InchiKey: FEOIEIQLXALHPJ-UHFFFAOYSA-N
Formula: C9H10N2
SMILES: CN(C)c1cccc(C#N)c1
Mol. weight [g/mol]: 146.19
CAS: 38803-30-4

Physical Properties

Property code	Value	Unit	Source
affp	894.60	kJ/mol	NIST Webbook
basg	868.10	kJ/mol	NIST Webbook
gf	371.64	kJ/mol	Joback Method
hf	228.38	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.624		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	551.50	K	Joback Method
tc	776.47	K	Joback Method
tf	327.59	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.92	J/mol×K	551.50	Joback Method
cpg	288.92	J/mol×K	588.99	Joback Method
cpg	300.13	J/mol×K	626.49	Joback Method
cpg	310.57	J/mol×K	663.98	Joback Method
cpg	320.28	J/mol×K	701.48	Joback Method
cpg	329.31	J/mol×K	738.97	Joback Method
cpg	337.70	J/mol×K	776.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38803304&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

affp:	Proton affinity
basg:	Gas basicity
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