

Iron, («eta»5-2,4-cyclopentadien-1-yl)(«eta»5-1H-pyrrolo

Other names:	Azaferrocene Cyclopentadienyl(pyrrolyl)iron
Inchi:	InChI=1S/C5H5.C4H4N.Fe/c2*1-2-4-5-3-1;/h1-5H;1-4H;/q;-1;+1
InchiKey:	MQFBMPWNHOLGOH-UHFFFAOYSA-N
Formula:	C9H9FeN
SMILES:	C12C3C4C5C1[Fe]23451678C2C1C6N7C28
Mol. weight [g/mol]:	187.02
CAS:	11077-12-6

Physical Properties

Property code	Value	Unit	Source
ie	7.20 ± 0.10	eV	NIST Webbook
ss	211.80	J/mol×K	NIST Webbook
ss	170.30	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	183.40	J/mol×K	298.15	NIST Webbook
cps	177.00	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C11077126&Units=SI>

Legend

cps: Solid phase heat capacity

ie: Ionization energy
ss: Solid phase molar entropy at standard conditions

Latest version available from:

<https://www.cheméo.com/cid/73-386-3/Iron-eta-5-2-4-cyclopentadien-1-yl-eta-5-1H-pyrrol-1-yl.pdf>

Generated by Cheméo on 2024-04-29 12:48:53.137965901 +0000 UTC m=+16684182.058543216.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.