2-Ethynylpyridine

Inchi: InChI=1S/C7H5N/c1-2-7-5-3-4-6-8-7/h1,3-6H
InchiKey: NHUBNHMFXQNNMV-UHFFFAOYSA-N
Formula: C7H5N
SMILES: C#Cc1ccccn1
Mol. weight [g/mol]: 103.12

Physical Properties

Property code	Value	Unit	Source
af	0.2725		Cheméo Relay (1.0)
gf	364.27	kJ/mol	Cheméo Relay (1.0, beta)
hf	382.98	kJ/mol	Cheméo Relay (1.0)
hvap	47.47	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-0.24		Cheméo Relay (1.0)
logp	1.063		Crippen Method
mcvol	87.110	ml/mol	McGowan Method
pc	5084.10	kPa	Cheméo Relay (1.0, beta)
tb	439.42	K	Cheméo Relay (1.0)
tc	674.22	K	Cheméo Relay (1.0)
tf	267.83	K	Cheméo Relay (1.0)
vc	0.301	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.50 ± 0.50	K	1.90	NIST Webbook
tbrp	358.00	K	4.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1945842&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume