5-Cyano-1-pentyne

Other names: 5-Cyano-1-pentyne
5-cyanopent-1-yne
Inchi: InChI=1S/C6H7N/c1-2-3-4-5-6-7/h1H,3-5H2
InchiKey: JZYKFLLRVPPISG-UHFFFAOYSA-N
Formula: C6H7N
SMILES: C#CCCCC#N
Mol. weight [g/mol]: 93.13

Physical Properties

Property code	Value	Unit	Source
af	0.3737		Cheméo Relay (1.0)
hf	257.88	kJ/mol	Cheméo Relay (1.0)
hfus	15.78	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Cheméo Relay (1.0)
ie	10.87	eV	Cheméo Relay (1.0)
log10ws	-1.12		Cheméo Relay (1.0)
logp	1.313		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	472.58	K	Cheméo Relay (1.0)
tc	658.21	K	Cheméo Relay (1.0)
tf	225.41	K	Cheméo Relay (1.0)
vc	0.317	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.56	J/mol×K	428.88	Joback Method
cpg	169.98	J/mol×K	462.70	Joback Method
cpg	177.02	J/mol×K	496.53	Joback Method
cpg	183.68	J/mol×K	530.35	Joback Method
cpg	190.01	J/mol×K	564.18	Joback Method
cpg	195.99	J/mol×K	598.00	Joback Method
cpg	201.67	J/mol×K	631.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.00 ± 1.00	K	14.90	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=C14918219&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume