Senecionitrile

Other names: Senecionitrile
Inchi: InChI=1S/C5H7N/c1-5(2)3-4-6/h3H,1-2H3
InchiKey: AUGKLUNRHYPDAM-UHFFFAOYSA-N
Formula: C5H7N
SMILES: CC(C)=CC#N
Mol. weight [g/mol]: 81.12

Physical Properties

Property code	Value	Unit	Source
hfus	9.10	kJ/mol	Joback Method
ie	9.65	eV	Cheméo Relay (1.0)
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
rinpol	770.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.79	J/mol×K	419.92	Joback Method
cpg	144.32	J/mol×K	454.03	Joback Method
cpg	151.44	J/mol×K	488.14	Joback Method
cpg	158.15	J/mol×K	522.25	Joback Method
cpg	164.50	J/mol×K	556.36	Joback Method
cpg	170.49	J/mol×K	590.47	Joback Method
cpg	176.15	J/mol×K	624.57	Joback Method

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=C4786247&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices