

1-Pentamine, n-ethyl-

Other names:	Pentylamine, N-ethyl- N-Ethylpentylamine ethylamyl-amine
Inchi:	InChI=1S/C7H17N/c1-3-5-6-7-8-4-2/h8H,3-7H2,1-2H3
InchiKey:	ICVFPLUSMYSIFO-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCCCNCC
Mol. weight [g/mol]:	115.22

Physical Properties

Property code	Value	Unit	Source
af	0.4399		Cheméo Relay (1.0)
gf	97.45	kJ/mol	Joback Method
hf	-136.20	kJ/mol	Cheméo Relay (1.0)
hfus	18.98	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-0.99		Cheméo Relay (1.0)
logp	1.786		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	855.00		NIST Webbook
tb	410.67	K	Cheméo Relay (1.0)
tc	568.91	K	Cheméo Relay (1.0)
tf	215.41	K	Cheméo Relay (1.0)
vc	0.456	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.17	J/mol×K	409.73	Joback Method
cpg	250.74	J/mol×K	437.93	Joback Method
cpg	262.84	J/mol×K	466.14	Joback Method
cpg	274.48	J/mol×K	494.34	Joback Method

cpg	285.67	J/mol×K	522.55	Joback Method
cpg	296.42	J/mol×K	550.75	Joback Method
cpg	306.74	J/mol×K	578.95	Joback Method

Sources

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=C17839268&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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