1-PENTANAMINE, N,N-DIMETHYL-

Inchi: InChI=1S/C7H17N/c1-4-5-6-7-8(2)3/h4-7H2,1-3H3
InchiKey: IDFANOPDMXWIOP-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCCCCN(C)C
Mol. weight [g/mol]: 115.22

Physical Properties

Property code	Value	Unit	Source
af	0.3781		Cheméo Relay (1.0)
gf	118.84	kJ/mol	Joback Method
hf	-113.96	kJ/mol	Cheméo Relay (1.0)
hfus	16.91	kJ/mol	Joback Method
hvap	37.76	kJ/mol	Cheméo Relay (1.0)
ie	7.99	eV	Cheméo Relay (1.0)
log10ws	-1.21		Cheméo Relay (1.0)
logp	1.738		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	795.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	761.30		NIST Webbook
tb	395.65 ± 3.00	K	NIST Webbook
tb	395.15 ± 3.00	K	NIST Webbook
tc	556.76	K	Cheméo Relay (1.0)
tf	176.40	K	Cheméo Relay (1.0)
vc	0.464	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.39	J/mol×K	372.00	Joback Method
cpg	234.38	J/mol×K	399.09	Joback Method
cpg	246.88	J/mol×K	426.18	Joback Method
cpg	258.89	J/mol×K	453.28	Joback Method

cpg	270.43	J/mol×K	480.37	Joback Method
cpg	281.51	J/mol×K	507.46	Joback Method
cpg	292.14	J/mol×K	534.55	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=C26153888&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