

Nanofin

Other names:	Piperidine, 2,6-dimethyl- 2,6-Lupetidine Lupetidin Lupetidine Naniopinum Nanophin Nanophine Nanophyn 2,6-Dimethylpiperidine NSC 63890
Inchi:	InChI=1S/C7H15N/c1-6-4-3-5-7(2)8-6/h6-8H,3-5H2,1-2H3
InchiKey:	SDGKUVSVPIIUCF-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CC1CCCC(C)N1
Mol. weight [g/mol]:	113.20
CAS:	504-03-0

Physical Properties

Property code	Value	Unit	Source
gf	112.51	kJ/mol	Joback Method
hf	-116.02	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	38.05	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.537		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	833.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	873.00		NIST Webbook
ripol	1016.00		NIST Webbook
ripol	1009.00		NIST Webbook
tb	400.45 ± 0.30	K	NIST Webbook
tb	401.00 ± 0.70	K	NIST Webbook
tc	634.06	K	Joback Method
tf	209.55 ± 0.30	K	NIST Webbook
vc	0.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.41	J/mol×K	422.99	Joback Method
cpg	232.27	J/mol×K	458.17	Joback Method
cpg	248.40	J/mol×K	493.35	Joback Method
cpg	263.82	J/mol×K	528.52	Joback Method
cpg	278.51	J/mol×K	563.70	Joback Method
cpg	292.50	J/mol×K	598.88	Joback Method
cpg	305.78	J/mol×K	634.06	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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