4,4-Dimethyl-piperidine

Other names: Piperidine, 4,4-dimethyl-
Inchi: InChI=1S/C7H15N/c1-7(2)3-5-8-6-4-7/h8H,3-6H2,1-2H3
InchiKey: IECMOFZIMWVOAS-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CC1(C)CCNCC1
Mol. weight [g/mol]: 113.20
CAS: 4045-30-1

Physical Properties

Property code	Value	Unit	Source
gf	114.73	kJ/mol	Joback Method
hf	-80.44	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	37.21	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.396		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	882.00		NIST Webbook
tb	418.70	K	NIST Webbook
tc	649.20	K	Joback Method
tf	304.96	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.01	J/mol×K	427.90	Joback Method
cpg	233.15	J/mol×K	464.78	Joback Method
cpg	249.12	J/mol×K	501.67	Joback Method
cpg	264.03	J/mol×K	538.55	Joback Method
cpg	278.00	J/mol×K	575.43	Joback Method
cpg	291.12	J/mol×K	612.32	Joback Method
cpg	303.49	J/mol×K	649.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	304.20	K	1.60	NIST Webbook

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=C4045301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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