Piperidine, 2,6-dimethyl-, (2R,6S)-rel-

Other names: Cis- 2,6-Dimethylpiperidine
2,6-Dimethylpiperidine
Inchi: InChI=1S/C7H15N/c1-6-4-3-5-7(2)8-6/h6-8H,3-5H2,1-2H3/t6-,7+
InchiKey: SDGKUVSVPIIUCF-KNVOCYPGSA-N
Formula: C7H15N
SMILES: CC1CCCC(C)N1
Mol. weight [g/mol]: 113.20
CAS: 766-17-6

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	41.30 ± 0.10	kJ/mol	NIST Webbook
hvap	42.40 ± 0.60	kJ/mol	NIST Webbook
ie	7.93 ± 0.05	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.537		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	422.99	K	Joback Method
tc	634.06	K	Joback Method
tf	276.82	K	Joback Method
vc	0.397	m3/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
hvapt	39.70 ± 0.10	kJ/mol	330.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	102.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C766176&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume