cis-2,5-dimethylpiperazine

Inchi: InChI=1S/C6H14N2/c1-5-3-8-6(2)4-7-5/h5-8H,3-4H2,1-2H3/t5-,6-/m1/s1
InchiKey: NSMWYRLQHIXVAP-PHDIDXHHSA-N
Formula: C6H14N2
SMILES: CC1CNC(C)CN1
Mol. weight [g/mol]: 114.19
CAS: 6284-84-0

Physical Properties

Property code	Value	Unit	Source
gf	191.80	kJ/mol	Joback Method
hf	-57.57	kJ/mol	Joback Method
hfus	23.38	kJ/mol	Joback Method
hvap	42.59	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	-0.044		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	448.66	K	Joback Method
tc	670.21	K	Joback Method
tf	292.05 ± 0.20	K	NIST Webbook
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.08	J/mol×K	448.66	Joback Method
cpg	232.09	J/mol×K	485.59	Joback Method
cpg	247.43	J/mol×K	522.51	Joback Method
cpg	262.10	J/mol×K	559.44	Joback Method
cpg	276.10	J/mol×K	596.36	Joback Method
cpg	289.42	J/mol×K	633.29	Joback Method
cpg	302.05	J/mol×K	670.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27253e+01
Coeff. B	-3.15983e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	316.17
Temperature range (K), max.	488.33

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6284840&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume