2,5-DIMETHYL-2,5-HEXANEDIAMINE

Other names: 2,5-dimethylhexane-2,5-diamine
Inchi: InChI=1S/C8H20N2/c1-7(2,9)5-6-8(3,4)10/h5-6,9-10H2,1-4H3
InchiKey: JWTVQZQPKHXGFM-UHFFFAOYSA-N
Formula: C8H20N2
SMILES: CC(C)(N)CCC(C)(C)N
Mol. weight [g/mol]: 144.26
CAS: 23578-35-0

Physical Properties

Property code	Value	Unit	Source
hf	-185.92	kJ/mol	Cheméo Relay (1.0)
hfus	12.04	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
logp	1.241		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	446.02	K	Cheméo Relay (1.0)
tc	640.36	K	Cheméo Relay (1.0)
tf	287.44	K	Cheméo Relay (1.0)
vc	0.542	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.06	J/mol×K	521.04	Joback Method
cpg	375.99	J/mol×K	556.45	Joback Method
cpg	390.86	J/mol×K	591.86	Joback Method
cpg	404.72	J/mol×K	627.28	Joback Method
cpg	417.66	J/mol×K	662.69	Joback Method
cpg	429.72	J/mol×K	698.10	Joback Method
cpg	440.99	J/mol×K	733.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33675e+01
Coeff. B	-3.65560e+03
Coeff. C	-6.82380e+01
Temperature range (K), min.	325.15
Temperature range (K), max.	522.01

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23578350&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume