

N-ISOPROPYL-1,3-PROPANEDIAMINE

Other names:	1,3-Propanediamine, N-isopropyl- N-Isopropyl-1,3-propylenediamine N-Isopropyltrimethylenediamine N-isopropylpropane-1,3-diamine
Inchi:	InChI=1S/C6H16N2/c1-6(2)8-5-3-4-7/h6,8H,3-5,7H2,1-2H3
InchiKey:	KFDIDIKKNMZLRZ-UHFFFAOYSA-N
Formula:	C6H16N2
SMILES:	CC(C)NCCCN
Mol. weight [g/mol]:	116.21
CAS:	3360-16-5

Physical Properties

Property code	Value	Unit	Source
hf	-122.04	kJ/mol	Cheméo Relay (1.0)
hfus	18.07	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Cheméo Relay (1.0)
logp	0.333		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
tb	435.20	K	NIST Webbook
tc	605.35	K	Cheméo Relay (1.0)
tf	241.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.54	J/mol×K	458.94	Joback Method
cpg	266.91	J/mol×K	490.24	Joback Method
cpg	278.73	J/mol×K	521.54	Joback Method
cpg	290.02	J/mol×K	552.84	Joback Method
cpg	300.80	J/mol×K	584.14	Joback Method
cpg	311.08	J/mol×K	615.44	Joback Method
cpg	320.87	J/mol×K	646.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56635e+01
Coeff. B	-4.12072e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	330.12
Temperature range (K), max.	460.18

Sources

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):	
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=C3360165&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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