

N,N'-DIISOPROPYL-1,3-PROPANEDIAMINE

Inchi:	InChI=1S/C9H22N2/c1-8(2)10-6-5-7-11-9(3)4/h8-11H,5-7H2,1-4H3
InchiKey:	OAVPQXXPJZPXTA-UHFFFAOYSA-N
Formula:	C9H22N2
SMILES:	CC(C)NCCCNC(C)C
Mol. weight [g/mol]:	158.29
CAS:	63737-71-3

Physical Properties

Property code	Value	Unit	Source
hf	-179.04	kJ/mol	Cheméo Relay (1.0)
hfus	22.22	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Cheméo Relay (1.0)
logp	1.373		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
tb	461.04	K	Cheméo Relay (1.0)
tc	625.19	K	Cheméo Relay (1.0)
tf	258.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.18	J/mol×K	504.78	Joback Method
cpg	390.72	J/mol×K	534.38	Joback Method
cpg	405.60	J/mol×K	563.98	Joback Method
cpg	419.82	J/mol×K	593.58	Joback Method
cpg	433.40	J/mol×K	623.17	Joback Method
cpg	446.37	J/mol×K	652.77	Joback Method
cpg	458.74	J/mol×K	682.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41216e+01
Coeff. B	-4.08536e+03
Coeff. C	-7.66680e+01
Temperature range (K), min.	371.98
Temperature range (K), max.	540.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63737713&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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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