

N-(n-Propyl)-1,3-propanediamine

Other names:	1,3-Propanediamine, N-propyl- 1-Amino-3-(propylamino)propane 3-n-Propylaminopropylamine N-(n-Propyl)-1,3-trimethylenediamine N-Propyl-1,3-propanediamine N-propylpropane-1,3-diamine
Inchi:	InChI=1S/C6H16N2/c1-2-5-8-6-3-4-7/h8H,2-7H2,1H3
InchiKey:	OWKYZAGJTTTXOK-UHFFFAOYSA-N
Formula:	C6H16N2
SMILES:	CCCNCCCN
Mol. weight [g/mol]:	116.20
CAS:	23764-31-0

Physical Properties

Property code	Value	Unit	Source
gf	155.48	kJ/mol	Joback Method
hf	-79.91	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.335		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	442.20	K	NIST Webbook
tc	643.08	K	Joback Method
tf	293.30	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.40	J/mol×K	459.38	Joback Method
cpg	266.42	J/mol×K	490.00	Joback Method
cpg	277.93	J/mol×K	520.61	Joback Method

cpg	288.93	J/mol×K	551.23	Joback Method
cpg	299.45	J/mol×K	581.85	Joback Method
cpg	309.49	J/mol×K	612.46	Joback Method
cpg	319.08	J/mol×K	643.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56669e+01
Coeff. B	-4.17783e+03
Coeff. C	-6.40680e+01
Temperature range (K), min.	335.72
Temperature range (K), max.	467.51

Sources

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=C23764310&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

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

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