

Di-n-propylethylamine

Other names:	1-Propanamine, N-ethyl-N-propyl-
Inchi:	InChI=1S/C8H19N/c1-4-7-9(6-3)8-5-2/h4-8H2,1-3H3
InchiKey:	XWCCTMBMQUCLSI-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCN(CC)CCC
Mol. weight [g/mol]:	129.25

Physical Properties

Property code	Value	Unit	Source
af	0.4073		Cheméo Relay (1.0)
gf	127.26	kJ/mol	Joback Method
hf	-150.90	kJ/mol	Cheméo Relay (1.0)
hfus	19.50	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Cheméo Relay (1.0)
ie	7.71	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	2.128		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	836.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	838.00		NIST Webbook
tb	402.15 ± 3.00	K	NIST Webbook
tb	404.15 ± 3.00	K	NIST Webbook
tc	560.18	K	Cheméo Relay (1.0)
tf	169.32	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.25	J/mol×K	394.88	Joback Method
cpg	275.33	J/mol×K	421.93	Joback Method
cpg	288.87	J/mol×K	448.98	Joback Method

cpg	301.88	J/mol×K	476.04	Joback Method
cpg	314.38	J/mol×K	503.09	Joback Method
cpg	326.38	J/mol×K	530.14	Joback Method
cpg	337.90	J/mol×K	557.19	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20634928&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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