

1-UNDECANAMINE, N,N-DIMETHYL-

Inchi:	InChI=1S/C13H29N/c1-4-5-6-7-8-9-10-11-12-13-14(2)3/h4-13H2,1-3H3
InchiKey:	MMWFTWUMBYZIRZ-UHFFFAOYSA-N
Formula:	C13H29N
SMILES:	CCCCCCCCCCCN(C)C
Mol. weight [g/mol]:	199.38

Physical Properties

Property code	Value	Unit	Source
af	0.6246		Cheméo Relay (1.0)
gf	169.36	kJ/mol	Joback Method
hf	-248.28	kJ/mol	Cheméo Relay (1.0)
hfus	32.45	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-4.63		Cheméo Relay (1.0)
logp	4.079		Crippen Method
mcvol	204.010	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	517.66	K	Cheméo Relay (1.0)
tc	675.58	K	Cheméo Relay (1.0)
tf	257.84	K	Cheméo Relay (1.0)
vc	0.813	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.85	J/mol×K	509.28	Joback Method
cpg	509.86	J/mol×K	535.80	Joback Method
cpg	527.16	J/mol×K	562.33	Joback Method
cpg	543.77	J/mol×K	588.85	Joback Method
cpg	559.71	J/mol×K	615.38	Joback Method
cpg	575.00	J/mol×K	641.90	Joback Method
cpg	589.66	J/mol×K	668.43	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=C17373283&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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