

2-Ethylhexylamine, N,N-di(allyl)-

Inchi:	InChI=1S/C14H27N/c1-5-9-10-14(8-4)13-15(11-6-2)12-7-3/h6-7,14H,2-3,5,8-13H2,1,4H3
InchiKey:	PKRVTDDDDDQCHKM-UHFFFAOYSA-N
Formula:	C14H27N
SMILES:	C=CCN(CC=C)CC(CC)CCCC
Mol. weight [g/mol]:	209.37

Physical Properties

Property code	Value	Unit	Source
gf	351.02	kJ/mol	Joback Method
hf	-19.18	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	47.07	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.877		Crippen Method
mcvol	209.500	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
tb	525.08	K	Joback Method
tc	691.75	K	Joback Method
tf	261.49	K	Joback Method
vc	0.793	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.24	J/mol×K	525.08	Joback Method
cpg	522.35	J/mol×K	552.86	Joback Method
cpg	539.66	J/mol×K	580.64	Joback Method
cpg	556.19	J/mol×K	608.41	Joback Method
cpg	571.97	J/mol×K	636.19	Joback Method
cpg	587.03	J/mol×K	663.97	Joback Method
cpg	601.40	J/mol×K	691.75	Joback Method

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=U416171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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