

Heptylamine, N,N-di(allyl)-

Inchi:	InChI=1S/C13H25N/c1-4-7-8-9-10-13-14(11-5-2)12-6-3/h5-6H,2-4,7-13H2,1H3
InchiKey:	HPLMOJKLLLDPIG-UHFFFAOYSA-N
Formula:	C13H25N
SMILES:	C=CCN(CC=C)CCCCCCC
Mol. weight [g/mol]:	195.34

Physical Properties

Property code	Value	Unit	Source
gf	345.04	kJ/mol	Joback Method
hf	6.74	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	45.23	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.631		Crippen Method
mcvol	195.410	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1362.00		NIST Webbook
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tb	502.64	K	Joback Method
tc	667.20	K	Joback Method
tf	265.22	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.96	J/mol×K	502.64	Joback Method
cpg	471.13	J/mol×K	530.07	Joback Method
cpg	487.55	J/mol×K	557.49	Joback Method
cpg	503.24	J/mol×K	584.92	Joback Method
cpg	518.24	J/mol×K	612.35	Joback Method
cpg	532.57	J/mol×K	639.78	Joback Method
cpg	546.25	J/mol×K	667.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U416172&Units=SI

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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