

Isopropylamine, n-allyl-

Inchi:	InChI=1S/C6H13N/c1-4-5-7-6(2)3/h4,6-7H,1,5H2,2-3H3
InchiKey:	OWUBKHTYXCOYMM-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	C=CCNC(C)C
Mol. weight [g/mol]:	99.17
CAS:	35000-22-7

Physical Properties

Property code	Value	Unit	Source
gf	174.43	kJ/mol	Joback Method
hf	6.45	kJ/mol	Joback Method
hfus	11.59	kJ/mol	Joback Method
hvap	34.33	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.170		Crippen Method
mcvol	101.080	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	383.09	K	Joback Method
tc	560.60	K	Joback Method
tf	193.28	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.73	J/mol×K	383.09	Joback Method
cpg	195.89	J/mol×K	412.67	Joback Method
cpg	206.58	J/mol×K	442.26	Joback Method
cpg	216.82	J/mol×K	471.84	Joback Method
cpg	226.61	J/mol×K	501.43	Joback Method
cpg	235.97	J/mol×K	531.01	Joback Method
cpg	244.92	J/mol×K	560.60	Joback Method

Sources

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=C35000227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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