Allylethylamine

Other names: Allylethylamine
N-ethylallylamine
Inchi: InChI=1S/C5H11N/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3
InchiKey: PUUULGNNRPBVBA-UHFFFAOYSA-N
Formula: C5H11N
SMILES: C=CCNCC
Mol. weight [g/mol]: 85.15

Physical Properties

Property code	Value	Unit	Source
af	0.2870		Cheméo Relay (1.0)
gf	168.45	kJ/mol	Joback Method
hf	44.04	kJ/mol	Cheméo Relay (1.0)
hfus	12.53	kJ/mol	Joback Method
hvap	40.07	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	0.25		Cheméo Relay (1.0)
logp	0.782		Crippen Method
mcvol	86.990	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
tb	353.06	K	Cheméo Relay (1.0)
tc	511.07	K	Cheméo Relay (1.0)
tf	166.60	K	Cheméo Relay (1.0)
vc	0.308	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.09	J/mol×K	360.65	Joback Method
cpg	158.57	J/mol×K	389.62	Joback Method
cpg	167.67	J/mol×K	418.60	Joback Method
cpg	176.39	J/mol×K	447.57	Joback Method

cpg	184.75	J/mol×K	476.54	Joback Method
cpg	192.75	J/mol×K	505.52	Joback Method
cpg	200.41	J/mol×K	534.49	Joback Method

Sources

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=C2424024&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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