Aletamine

Other names:	«alpha»-Allylphenethylamine
	Alfetamine
	Benzeneethanamine, «alpha»-2-propenyl-
	«alpha»-2-Propenyl benzeneethanamine
Inchi:	InChI=1S/C11H15N/c1-2-6-11(12)9-10-7-4-3-5-8-10/h2-5,7-8,11H,1,6,9,12H2
InchiKey:	WQKXQJYCZMWOSD-UHFFFAOYSA-N
Formula:	C11H15N
SMILES:	C=CCC(N)Cc1ccccc1
Mol. weight [g/mol]:	161.24
CAS:	4255-23-6

Physical Properties

Property code	Value	Unit	Source
gf	306.00	kJ/mol	Joback Method
hf	120.10	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.133		Crippen Method
mcvol	147.770	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1311.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1814.00		NIST Webbook
tb	546.53	K	Joback Method
tc	768.13	K	Joback Method
tf	306.65	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.55	J/mol×K	546.53	Joback Method
cpg	359.08	J/mol×K	583.46	Joback Method
cpg	373.60	J/mol×K	620.40	Joback Method
cpg	387.15	J/mol×K	657.33	Joback Method
cpg	399.78	J/mol×K	694.26	Joback Method
cpg	411.56	J/mol×K	731.20	Joback Method
cpg	422.54	J/mol×K	768.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4255236&Units=SI
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

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