

azacyclotridecane

Inchi:	InChI=1S/C12H25N/c1-2-4-6-8-10-12-13-11-9-7-5-3-1/h13H,1-12H2
InchiKey:	UFADJPZTTUWZMP-UHFFFAOYSA-N
Formula:	C12H25N
SMILES:	C1CCCCCNCCCCC1
Mol. weight [g/mol]:	183.33
CAS:	295-03-4

Physical Properties

Property code	Value	Unit	Source
gf	85.33	kJ/mol	Joback Method
hf	-221.66	kJ/mol	Joback Method
hfus	12.49	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.491		Crippen Method
mcvol	179.060	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	576.62	K	Joback Method
tc	830.08	K	Joback Method
tf	317.01	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.95	J/molxK	576.62	Joback Method
cpg	488.66	J/molxK	618.86	Joback Method
cpg	515.52	J/molxK	661.11	Joback Method
cpg	540.51	J/molxK	703.35	Joback Method
cpg	563.60	J/molxK	745.59	Joback Method
cpg	584.75	J/molxK	787.84	Joback Method
cpg	603.93	J/molxK	830.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.00	K	3.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C295034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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