

Benzenepentamine

Inchi:	InChI=1S/C11H17N/c12-10-6-2-5-9-11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-6,9-10,12H2
InchiKey:	CGNLNKFBSBFJHY-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	NCCCCCc1ccccc1
Mol. weight [g/mol]:	163.26
CAS:	17734-21-3

Physical Properties

Property code	Value	Unit	Source
gf	220.60	kJ/mol	Joback Method
hf	-0.05	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	53.00	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.358		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	550.29	K	Joback Method
tc	762.50	K	Joback Method
tf	323.41	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.70	J/mol×K	550.29	Joback Method
cpg	378.46	J/mol×K	585.66	Joback Method
cpg	393.28	J/mol×K	621.03	Joback Method
cpg	407.21	J/mol×K	656.39	Joback Method
cpg	420.28	J/mol×K	691.76	Joback Method
cpg	432.53	J/mol×K	727.13	Joback Method
cpg	444.02	J/mol×K	762.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17734213&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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