

Pentyl isobutyl amine

Other names:	isobutyl-n-amyl-amine
Inchi:	InChI=1S/C9H21N/c1-4-5-6-7-10-8-9(2)3/h9-10H,4-8H2,1-3H3
InchiKey:	DZAGFVTUFXZPNP-UHFFFAOYSA-N
Formula:	C9H21N
SMILES:	CCCCCNCC(C)C
Mol. weight [g/mol]:	143.27

Physical Properties

Property code	Value	Unit	Source
gf	111.85	kJ/mol	Joback Method
hf	-180.90	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.422		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	996.00		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1115.00		NIST Webbook
tb	455.05	K	Joback Method
tc	625.99	K	Joback Method
tf	228.85	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.80	J/molxK	455.05	Joback Method
cpg	337.76	J/molxK	483.54	Joback Method
cpg	352.13	J/molxK	512.03	Joback Method
cpg	365.92	J/molxK	540.52	Joback Method
cpg	379.16	J/molxK	569.01	Joback Method

cpg	391.84	J/mol×K	597.50	Joback Method
cpg	404.00	J/mol×K	625.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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