

N-2-Butylamphetamine

Other names:	N-sec-Butylamphetamine
Inchi:	InChI=1S/C13H21N/c1-4-11(2)14-12(3)10-13-8-6-5-7-9-13/h5-9,11-12,14H,4,10H2,1-3H3
InchiKey:	FRERPLIKKJVMIL-UHFFFAOYSA-N
Formula:	C13H21N
SMILES:	CCC(C)NC(C)Cc1ccccc1
Mol. weight [g/mol]:	191.31

Physical Properties

Property code	Value	Unit	Source
gf	255.50	kJ/mol	Joback Method
hf	-32.21	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	52.47	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.006		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1635.00		NIST Webbook
tb	572.81	K	Joback Method
tc	778.60	K	Joback Method
tf	285.35	K	Joback Method
vc	0.678	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.47	J/mol×K	572.81	Joback Method

cpg	466.52	J/mol×K	607.11	Joback Method
cpg	483.53	J/mol×K	641.41	Joback Method
cpg	499.53	J/mol×K	675.70	Joback Method
cpg	514.58	J/mol×K	710.00	Joback Method
cpg	528.70	J/mol×K	744.30	Joback Method
cpg	541.96	J/mol×K	778.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R18240&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

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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