N-Methyl-N-n-butyl-amphetamine

Other names: N-Methyl-N-butylamphetamine
Inchi: InChI=1S/C14H23N/c1-4-5-11-15(3)13(2)12-14-9-7-6-8-10-14/h6-10,13H,4-5,11-12H2,1-
InchiKey: XWUXLSYHMHHYPV-UHFFFAOYSA-N
Formula: C14H23N
SMILES: CCCCN(C)C(C)Cc1ccccc1
Mol. weight [g/mol]: 205.34

Physical Properties

Property code	Value	Unit	Source
gf	287.75	kJ/mol	Joback Method
hf	-33.51	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.349		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1743.00		NIST Webbook
tb	558.40	K	Joback Method
tc	753.95	K	Joback Method
tf	291.43	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.17	J/mol×K	558.40	Joback Method

cpg	498.19	J/mol×K	590.99	Joback Method
cpg	516.15	J/mol×K	623.58	Joback Method
cpg	533.10	J/mol×K	656.18	Joback Method
cpg	549.08	J/mol×K	688.77	Joback Method
cpg	564.13	J/mol×K	721.36	Joback Method
cpg	578.31	J/mol×K	753.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R18179&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