N-n-butylamphetamine

Other names: Butylamphetamine
Inchi: InChI=1S/C13H21N/c1-3-4-10-14-12(2)11-13-8-6-5-7-9-13/h5-9,12,14H,3-4,10-11H2,1-2
InchiKey: VIAVBPFRYASSKF-UHFFFAOYSA-N
Formula: C13H21N
SMILES: CCCCNC(C)Cc1ccccc1
Mol. weight [g/mol]: 191.31
CAS: 51799-33-8

Physical Properties

Property code	Value	Unit	Source
gf	257.94	kJ/mol	Joback Method
hf	-26.93	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	52.86	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.007		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1422.00		NIST Webbook
ripol	1732.00		NIST Webbook
tb	573.25	K	Joback Method
tc	774.87	K	Joback Method
tf	300.35	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.14	J/mol×K	573.25	Joback Method
cpg	465.77	J/mol×K	606.85	Joback Method
cpg	482.41	J/mol×K	640.46	Joback Method
cpg	498.09	J/mol×K	674.06	Joback Method
cpg	512.85	J/mol×K	707.66	Joback Method
cpg	526.75	J/mol×K	741.27	Joback Method

cpg	539.81	J/mol×K	774.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51799338&Units=SI

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