N,N-Di-n-butylamphetamine

Other names: N,N-Dibutylamphetamine
Inchi: InChI=1S/C17H29N/c1-4-6-13-18(14-7-5-2)16(3)15-17-11-9-8-10-12-17/h8-12,16H,4-7,1
InchiKey: NZYBJDSRVQRZDZ-UHFFFAOYSA-N
Formula: C17H29N
SMILES: CCCCN(CCCC)C(C)Cc1ccccc1
Mol. weight [g/mol]: 247.42

Physical Properties

Property code	Value	Unit	Source
gf	313.01	kJ/mol	Joback Method
hf	-95.43	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.520		Crippen Method
mcvol	236.610	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1902.00		NIST Webbook
tb	627.04	K	Joback Method
tc	815.70	K	Joback Method
tf	325.24	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.61	J/mol×K	627.04	Joback Method
cpg	658.63	J/mol×K	658.48	Joback Method
cpg	677.57	J/mol×K	689.93	Joback Method
cpg	695.48	J/mol×K	721.37	Joback Method
cpg	712.40	J/mol×K	752.81	Joback Method

cpg	728.38	J/mol×K	784.26	Joback Method
cpg	743.46	J/mol×K	815.70	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=R18197&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