N,N-Diethylamphetamine

Other names: Diethylamphetamine
Inchi: InChI=1S/C13H21N/c1-4-14(5-2)12(3)11-13-9-7-6-8-10-13/h6-10,12H,4-5,11H2,1-3H3
InchiKey: WZQLSNAODWITCK-UHFFFAOYSA-N
Formula: C13H21N
SMILES: CCN(CC)C(C)Cc1ccccc1
Mol. weight [g/mol]: 191.31
CAS: 51930-71-3

Physical Properties

Property code	Value	Unit	Source
gf	279.33	kJ/mol	Joback Method
hf	-12.87	kJ/mol	Joback Method
hfus	22.96	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.959		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	535.52	K	Joback Method
tc	733.75	K	Joback Method
tf	280.16	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.96	J/mol×K	535.52	Joback Method
cpg	447.51	J/mol×K	568.56	Joback Method

cpg	465.00	J/mol×K	601.60	Joback Method
cpg	481.50	J/mol×K	634.63	Joback Method
cpg	497.03	J/mol×K	667.67	Joback Method
cpg	511.66	J/mol×K	700.71	Joback Method
cpg	525.42	J/mol×K	733.75	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=C51930713&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