

3-Diethylaminobutyranilide

Other names:	Octacaine
Inchi:	InChI=1S/C14H22N2O/c1-4-16(5-2)12(3)11-14(17)15-13-9-7-6-8-10-13/h6-10,12H,4-5,1
InchiKey:	HKOURKRGAFKVFP-UHFFFAOYSA-N
Formula:	C14H22N2O
SMILES:	CCN(CC)C(C)CC(=O)Nc1ccccc1
Mol. weight [g/mol]:	234.34
CAS:	13912-77-1

Physical Properties

Property code	Value	Unit	Source
gf	248.22	kJ/mol	Joback Method
hf	-92.62	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.746		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1893.00		NIST Webbook
tb	662.44	K	Joback Method
tc	865.83	K	Joback Method
tf	394.02	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.63	J/molxK	662.44	Joback Method
cpg	578.36	J/molxK	696.34	Joback Method
cpg	594.05	J/molxK	730.24	Joback Method
cpg	608.74	J/molxK	764.13	Joback Method
cpg	622.48	J/molxK	798.03	Joback Method
cpg	635.33	J/molxK	831.93	Joback Method
cpg	647.33	J/molxK	865.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C13912771&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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