

N,N-DIETHYL-O-NITROANILINE

Inchi:	InChI=1S/C10H14N2O2/c1-3-11(4-2)9-7-5-6-8-10(9)12(13)14/h5-8H,3-4H2,1-2H3
InchiKey:	BUBRUAQVAPTGHV-UHFFFAOYSA-N
Formula:	C10H14N2O2
SMILES:	CCN(CC)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
hf	-2.01	kJ/mol	Cheméo Relay (1.0)
hfus	29.69	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Cheméo Relay (1.0)
ie	7.84	eV	Cheméo Relay (1.0)
log10ws	-3.75		Cheméo Relay (1.0)
logp	2.441		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
tb	556.31	K	Cheméo Relay (1.0)
tf	309.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.46	J/mol×K	624.14	Joback Method
cpg	408.90	J/mol×K	662.60	Joback Method
cpg	422.31	J/mol×K	701.06	Joback Method
cpg	434.76	J/mol×K	739.52	Joback Method
cpg	446.29	J/mol×K	777.98	Joback Method
cpg	456.97	J/mol×K	816.44	Joback Method
cpg	466.85	J/mol×K	854.90	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216173&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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