

Phenol, 4-dimethylamino, dimethylcarbamate (from Neostigmine Bromide)

Inchi:	InChI=1S/C11H16N2O2/c1-12(2)9-5-7-10(8-6-9)15-11(14)13(3)4/h5-8H,1-4H3
InchiKey:	GZKMLMDRMXOKGA-UHFFFAOYSA-N
Formula:	C11H16N2O2
SMILES:	CN(C)C(=O)Oc1ccc(N(C)C)cc1
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
gf	132.16	kJ/mol	Joback Method
hf	-155.05	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.813		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	583.91	K	Joback Method
tc	788.45	K	Joback Method
tf	389.77	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.72	J/molxK	583.91	Joback Method
cpg	432.96	J/molxK	618.00	Joback Method
cpg	447.29	J/molxK	652.09	Joback Method
cpg	460.74	J/molxK	686.18	Joback Method
cpg	473.35	J/molxK	720.27	Joback Method
cpg	485.14	J/molxK	754.36	Joback Method
cpg	496.15	J/molxK	788.45	Joback Method

Sources

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=R489380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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