Benzaldehyde, 4-(diethylamino)-

Other names:	4-(Diethylamino)benzaldehyde
	4-(N,N-Diethylamino)benzaldehyde
	Benzaldehyde, p-(diethylamino)-
	p-(Diethylamino)benzaldehyde
	p-Formyl-N,N-diethylaniline
Inchi:	InChI=1S/C11H15NO/c1-3-12(4-2)11-7-5-10(9-13)6-8-11/h5-9H,3-4H2,1-2H3
InchiKey:	MNFZZNNFORDXSV-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCN(CC)c1ccc(C=O)cc1
Mol. weight [g/mol]:	177.24
CAS:	120-21-8

Physical Properties

Property code	Value	Unit	Source
af	0.5523		Cheméo Relay (1.0)
gf	155.78	kJ/mol	Joback Method
hf	-108.13	kJ/mol	Cheméo Relay (1.0)
hfus	23.21	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Cheméo Relay (1.0)
ie	7.57	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
logp	2.345		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	551.76	K	Cheméo Relay (1.0)
tc	777.31	K	Cheméo Relay (1.0)
tf	314.00	K	NIST Webbook
tf	313.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	447.20	K	0.90	NIST Webbook
tbrp	447.00	K	0.90	NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.60080e+01
Coeff. B	1.00884e+00
Coeff. C	-6.44360e-04
Coeff. D	1.55600e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120218&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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