5-Diethylamino-2-pentanol

Other names: 2-Pentanol, 5-(diethylamino)-
5-diethylaminopentan-2-ol
Inchi: InChI=1S/C9H21NO/c1-4-10(5-2)8-6-7-9(3)11/h9,11H,4-8H2,1-3H3
InchiKey: OAQYRNDEOJQVBN-UHFFFAOYSA-N
Formula: C9H21NO
SMILES: CCN(CC)CCCC(C)O
Mol. weight [g/mol]: 159.27
CAS: 5412-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-3.58	kJ/mol	Joback Method
hf	-319.07	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	53.96	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.489		Crippen Method
mcvol	153.520	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	509.50	K	Joback Method
tc	670.38	K	Joback Method
tf	269.48	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.66	J/mol×K	509.50	Joback Method
cpg	382.06	J/mol×K	536.31	Joback Method
cpg	394.90	J/mol×K	563.13	Joback Method
cpg	407.22	J/mol×K	589.94	Joback Method
cpg	419.01	J/mol×K	616.75	Joback Method
cpg	430.31	J/mol×K	643.56	Joback Method
cpg	441.12	J/mol×K	670.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.00 ± 1.00	K	4.70	NIST Webbook
tbrp	370.00	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.12325e+01
Coeff. B	-3.20314e+03
Coeff. C	-7.36590e+01
Temperature range (K), min.	366.32
Temperature range (K), max.	614.64

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=C5412691&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume