

Leucinocaine

Other names:

1-Pentanol, 2-(diethylamino)-4-methyl-, p-aminobenzoate
2-(Diethylamino)-4-methyl-1-pentanol p-aminobenzoate
S.F. 147

Inchi:

2-(Diethylamino)-4-methyl-1-pentanol p-aminobenzoate (ester)

InchiKey:

MLHBDHJHNDJBLI-UHFFFAOYSA-N

Formula:

C₁₇H₂₈N₂O₂

SMILES:

CCN(CC)C(COC(=O)c1ccc(N)cc1)CC(C)C

Mol. weight [g/mol]:

292.42

CAS:

92-23-9

Physical Properties

Property code	Value	Unit	Source
gf	133.47	kJ/mol	Joback Method
hf	-323.19	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.182		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	780.40	K	Joback Method
tc	986.46	K	Joback Method
tf	478.18	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/mol×K	780.40	Joback Method
cpg	784.80	J/mol×K	814.74	Joback Method
cpg	800.50	J/mol×K	849.09	Joback Method

cpg	815.13	J/mol×K	883.43	Joback Method
cpg	828.73	J/mol×K	917.77	Joback Method
cpg	841.36	J/mol×K	952.12	Joback Method
cpg	853.04	J/mol×K	986.46	Joback Method

Sources

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=C92239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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