

Aniline, 3,4-diethoxy-

Inchi:	InChI=1S/C10H15NO2/c1-3-12-9-6-5-8(11)7-10(9)13-4-2/h5-7H,3-4,11H2,1-2H3
InchiKey:	IKYZLUA AOLUOFW-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CCOc1ccc(N)cc1OCC
Mol. weight [g/mol]:	181.23
CAS:	39052-12-5

Physical Properties

Property code	Value	Unit	Source
gf	-17.08	kJ/mol	Joback Method
hf	-266.79	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.066		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	582.21	K	Joback Method
tc	795.30	K	Joback Method
tf	381.64	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.65	J/molxK	582.21	Joback Method
cpg	378.45	J/molxK	617.72	Joback Method
cpg	391.58	J/molxK	653.24	Joback Method
cpg	404.04	J/molxK	688.75	Joback Method
cpg	415.81	J/molxK	724.27	Joback Method
cpg	426.90	J/molxK	759.78	Joback Method
cpg	437.30	J/molxK	795.30	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=C39052125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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