

4-AMINOBUTYRALDEHYDE DIETHYL ACETAL

Other names:	1-Butanamine, 4,4-diethoxy- 4-Aminobutyraldehyde diethyl ester 4,4-diethoxybutylamine
Inchi:	InChI=1S/C8H19NO2/c1-3-10-8(11-4-2)6-5-7-9/h8H,3-7,9H2,1-2H3
InchiKey:	GFLPSABXBDCMCN-UHFFFAOYSA-N
Formula:	C8H19NO2
SMILES:	CCOC(CCCN)OCC
Mol. weight [g/mol]:	161.25

Physical Properties

Property code	Value	Unit	Source
hfus	20.53	kJ/mol	Joback Method
logp	1.124		Crippen Method
mcvol	145.300	ml/mol	McGowan Method
tb	469.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.87	J/mol×K	499.37	Joback Method
cpg	356.37	J/mol×K	529.33	Joback Method
cpg	369.40	J/mol×K	559.29	Joback Method
cpg	381.96	J/mol×K	589.26	Joback Method
cpg	394.05	J/mol×K	619.22	Joback Method
cpg	405.66	J/mol×K	649.18	Joback Method
cpg	416.80	J/mol×K	679.14	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6346094&Units=SI>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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