4-Aminobutyraldehyde diethyl acetal

Other names: 1-Butanamine, 4,4-diethoxy-
4-Aminobutyralodehyde 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]: 161.24
CAS: 6346-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-129.51	kJ/mol	Joback Method
hf	-444.38	kJ/mol	Joback Method
hfus	20.53	kJ/mol	Joback Method
hvap	48.47	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.124		Crippen Method
mcvol	145.300	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	469.20	K	NIST Webbook
tc	679.14	K	Joback Method
tf	292.64	K	Joback Method
vc	0.542	m3/kmol	Joback Method

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

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=C6346094&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume