Anilinoacetaldehyde diethyl acetal

Inchi: InChI=1S/C12H19NO2/c1-3-14-12(15-4-2)10-13-11-8-6-5-7-9-11/h5-9,12-13H,3-4,10H2,
InchiKey: DHGUGEBXVGPRRD-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CCOC(CNc1ccccc1)OCC
Mol. weight [g/mol]: 209.28
CAS: 22758-34-5

Physical Properties

Property code	Value	Unit	Source
gf	39.52	kJ/mol	Joback Method
hf	-270.73	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.498		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
tb	595.21	K	Joback Method
tc	796.01	K	Joback Method
tf	333.54	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.21	J/mol×K	595.21	Joback Method
cpg	468.46	J/mol×K	628.68	Joback Method
cpg	483.85	J/mol×K	662.14	Joback Method
cpg	498.41	J/mol×K	695.61	Joback Method
cpg	512.13	J/mol×K	729.08	Joback Method
cpg	525.04	J/mol×K	762.54	Joback Method
cpg	537.14	J/mol×K	796.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22758345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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