N-Benzylaminoacetaldehyde diethylacetal

Inchi: InChI=1S/C13H21NO2/c1-3-15-13(16-4-2)11-14-10-12-8-6-5-7-9-12/h5-9,13-14H,3-4,10-
InchiKey: SXFVQTYQHWRYOS-UHFFFAOYSA-N
Formula: C13H21NO2
SMILES: CCOC(CNCc1ccccc1)OCC
Mol. weight [g/mol]: 223.32

Physical Properties

Property code	Value	Unit	Source
af	0.5598		Cheméo Relay (1.0)
gf	47.94	kJ/mol	Joback Method
hf	-320.03	kJ/mol	Cheméo Relay (1.0)
hfus	27.42	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-1.29		Cheméo Relay (1.0)
logp	2.175		Crippen Method
mcvol	191.990	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
tb	556.88	K	Cheméo Relay (1.0)
tc	728.86	K	Cheméo Relay (1.0)
tf	230.17	K	Cheméo Relay (1.0)
vc	0.694	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.25	J/mol×K	618.09	Joback Method
cpg	520.04	J/mol×K	651.10	Joback Method
cpg	535.93	J/mol×K	684.11	Joback Method
cpg	550.95	J/mol×K	717.12	Joback Method
cpg	565.11	J/mol×K	750.13	Joback Method
cpg	578.43	J/mol×K	783.14	Joback Method
cpg	590.91	J/mol×K	816.16	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61190101&Units=SI
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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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