N,N-Dimethylformamide dibenzylacetal

Other names: Methanamine, N,N-dimethyl-1,1-bis(phenylmethoxy)-
1,1-bis(benzyloxy)trimethylamine
Inchi: InChI=1S/C17H21NO2/c1-18(2)17(19-13-15-9-5-3-6-10-15)20-14-16-11-7-4-8-12-16/h3-
InchiKey: JFIKHFNGAURIIB-UHFFFAOYSA-N
Formula: C17H21NO2
SMILES: CN(C)C(OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 271.35
CAS: 2016-04-8

Physical Properties

Property code	Value	Unit	Source
gf	215.42	kJ/mol	Joback Method
hf	-123.34	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.265		Crippen Method
mcvol	224.590	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
tb	698.56	K	Joback Method
tc	919.54	K	Joback Method
tf	396.12	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.70	J/mol×K	698.56	Joback Method
cpg	638.98	J/mol×K	735.39	Joback Method
cpg	655.96	J/mol×K	772.22	Joback Method
cpg	671.68	J/mol×K	809.05	Joback Method
cpg	686.18	J/mol×K	845.88	Joback Method
cpg	699.53	J/mol×K	882.71	Joback Method
cpg	711.77	J/mol×K	919.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.00 ± 1.00	K	0.03	NIST Webbook
tbrp	404.50 ± 0.50	K	0.01	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2016048&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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