Diethylaminoacetone

Other names:	2-Propanone, 1-(diethylamino)- N,N-Diethylaminoacetone
Inchi:	InChI=1S/C7H15NO/c1-4-8(5-2)6-7(3)9/h4-6H2,1-3H3
InchiKey:	GDXMMBDEMOUTNS-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CCN(CC)CC(C)=O
Mol. weight [g/mol]:	129.20
CAS:	1620-14-0

Physical Properties

Property code	Value	Unit	Source
chl	-4617.30 ± 2.10	kJ/mol	NIST Webbook
gf	-10.08	kJ/mol	Joback Method
hf	-233.30 ± 2.20	kJ/mol	NIST Webbook
hfl	-281.00 ± 2.20	kJ/mol	NIST Webbook
hfus	18.51	kJ/mol	Joback Method
hvap	47.70 ± 0.30	kJ/mol	NIST Webbook
hvap	47.70 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.917		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	425.87	K	Joback Method
tc	600.81	K	Joback Method
tf	251.05	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.86	J/mol×K	425.87	Joback Method
cpg	257.29	J/mol×K	455.03	Joback Method
cpg	269.17	J/mol×K	484.18	Joback Method
cpg	280.54	J/mol×K	513.34	Joback Method

cpg	291.41	J/mol×K	542.50	Joback Method
cpg	301.79	J/mol×K	571.65	Joback Method
cpg	311.69	J/mol×K	600.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620140&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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