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

Physical Properties

Property code	Value	Unit	Source
af	0.4213		Cheméo Relay (1.0)
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
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	0.09		Cheméo Relay (1.0)
logp	0.917		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	435.39	K	Cheméo Relay (1.0)
tc	604.87	K	Cheméo Relay (1.0)
tf	232.07	K	Cheméo Relay (1.0)
vc	0.430	m3/kmol	Cheméo Relay (1.0)

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

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1620140&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume