3-Diethylamino-2,2-dimethylpropionaldehyde

Other names:	«alpha»,«alpha»-Dimethyl-«beta»-diethylaminopropionaldehyde
	Diethylaminopivalaldehyde
	Propanal, 3-(diethylamino)-2,2-dimethyl-
	Propionaldehyde, 3-(diethylamino)-2,2-dimethyl-
Inchi:	InChI=1S/C9H19NO/c1-5-10(6-2)7-9(3,4)8-11/h8H,5-7H2,1-4H3
InchiKey:	AAHIYAKUVPMLMX-UHFFFAOYSA-N
Formula:	C9H19NO
SMILES:	CCN(CC)CC(C)(C)C=O
Mol. weight [g/mol]:	157.25
CAS:	6343-47-1

Physical Properties

Property code	Value	Unit	Source
gf	39.00	kJ/mol	Joback Method
hf	-255.89	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.553		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	463.19	K	Joback Method
tc	641.53	K	Joback Method
tf	268.08	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.35	J/mol×K	463.19	Joback Method
cpg	348.56	J/mol×K	492.91	Joback Method
cpg	362.99	J/mol×K	522.64	Joback Method
cpg	376.67	J/mol×K	552.36	Joback Method
cpg	389.63	J/mol×K	582.09	Joback Method

cpg	401.91	J/mol×K	611.81	Joback Method
cpg	413.53	J/mol×K	641.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.50 ± 0.50	K	5.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6343471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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