3-Dimethylamino-2,2-dimethylpropionaldehyde

Other names: Propanal, 3-(dimethylamino)-2,2-dimethyl-
Inchi: InChI=1S/C7H15NO/c1-7(2,6-9)5-8(3)4/h6H,5H2,1-4H3
InchiKey: NYUOVICEZDPRBR-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CN(C)CC(C)(C)C=O
Mol. weight [g/mol]: 129.20
CAS: 15451-14-6

Physical Properties

Property code	Value	Unit	Source
gf	22.16	kJ/mol	Joback Method
hf	-214.61	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	38.64	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	0.773		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	416.00 ± 1.00	K	NIST Webbook
tc	598.64	K	Joback Method
tf	245.54	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.06	J/mol×K	417.43	Joback Method
cpg	261.50	J/mol×K	447.63	Joback Method
cpg	274.22	J/mol×K	477.83	Joback Method
cpg	286.25	J/mol×K	508.03	Joback Method
cpg	297.62	J/mol×K	538.24	Joback Method
cpg	308.37	J/mol×K	568.44	Joback Method
cpg	318.51	J/mol×K	598.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15451146&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume