N,N-Dimethylamino-2,4-pentadiene-5-al

Inchi: InChI=1S/C7H11NO/c1-8(2)6-4-3-5-7-9/h3-7H,1-2H3/b5-3+,6-4+
InchiKey: MJPXUXNGHKYZIV-GGWOSOGESA-N
Formula: C7H11NO
SMILES: CN(C)C=CC=CC=O
Mol. weight [g/mol]: 125.17
CAS: 4688-60-2

Physical Properties

Property code	Value	Unit	Source
chs	-4199.00 ± 1.00	kJ/mol	NIST Webbook
gf	179.76	kJ/mol	Joback Method
hf	-29.10	kJ/mol	NIST Webbook
hfus	19.60	kJ/mol	Joback Method
hsub	99.04 ± 0.92	kJ/mol	NIST Webbook
hvap	39.86	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.817		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	428.98	K	Joback Method
tc	616.55	K	Joback Method
tf	232.96	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.15	J/mol×K	428.98	Joback Method
cpg	226.62	J/mol×K	460.24	Joback Method
cpg	237.40	J/mol×K	491.50	Joback Method
cpg	247.53	J/mol×K	522.77	Joback Method
cpg	257.05	J/mol×K	554.03	Joback Method
cpg	266.00	J/mol×K	585.29	Joback Method
cpg	274.40	J/mol×K	616.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4688602&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

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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