N,N-Dimethylamino-2,4,6-heptatriene-7al

Inchi: InChI=1S/C9H13NO/c1-10(2)8-6-4-3-5-7-9-11/h3-9H,1-2H3/b4-3+,7-5+,8-6+
InchiKey: PIKCCROVFWBDJH-OKWWDJPNSA-N
Formula: C9H13NO
SMILES: CN(C)C=CC=CC=CO
Mol. weight [g/mol]: 151.21
CAS: 13044-92-3

Physical Properties

Property code	Value	Unit	Source
chs	-5289.80 ± 6.30	kJ/mol	NIST Webbook
gf	276.82	kJ/mol	Joback Method
hf	21.60	kJ/mol	NIST Webbook
hfus	24.98	kJ/mol	Joback Method
hsub	131.00 ± 1.00	kJ/mol	NIST Webbook
hvap	44.27	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.373		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	478.90	K	Joback Method
tc	671.61	K	Joback Method
tf	250.42	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.35	J/mol×K	478.90	Joback Method
cpg	294.32	J/mol×K	511.02	Joback Method
cpg	306.45	J/mol×K	543.14	Joback Method
cpg	317.81	J/mol×K	575.26	Joback Method
cpg	328.44	J/mol×K	607.38	Joback Method
cpg	338.40	J/mol×K	639.50	Joback Method
cpg	347.75	J/mol×K	671.61	Joback Method

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=C13044923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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