3«alpha»-Acetoxynortropane

Inchi: InChI=1S/C9H15NO2/c1-6(11)12-9-4-7-2-3-8(5-9)10-7/h7-10H,2-5H2,1H3/t7-,8+,9+
InchiKey: TZSPCFWIYSJTGI-BRPSZJMVSA-N
Formula: C9H15NO2
SMILES: CC(=O)OC1CC2CCC(C1)N2
Mol. weight [g/mol]: 169.22

Physical Properties

Property code	Value	Unit	Source
gf	-31.72	kJ/mol	Joback Method
hf	-323.14	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	51.40	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	0.833		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	547.51	K	Joback Method
tc	769.16	K	Joback Method
tf	392.98	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.70	J/mol×K	547.51	Joback Method
cpg	358.18	J/mol×K	584.45	Joback Method
cpg	374.64	J/mol×K	621.39	Joback Method
cpg	390.10	J/mol×K	658.33	Joback Method
cpg	404.61	J/mol×K	695.28	Joback Method
cpg	418.19	J/mol×K	732.22	Joback Method
cpg	430.89	J/mol×K	769.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R509543&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume