3-Nonen-5-one

Other names: Non-3-en-5-one
Inchi: InChI=1S/C9H16O/c1-3-5-7-9(10)8-6-4-2/h5,7H,3-4,6,8H2,1-2H3/b7-5+
InchiKey: FRMKAKWKXLDSSR-FNORWQNLSA-N
Formula: C9H16O
SMILES: CCC=CC(=O)CCCC
Mol. weight [g/mol]: 140.22
CAS: 82456-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-224.45	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	42.33	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1051.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1051.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1372.00		NIST Webbook
tb	463.35	K	Joback Method
tc	645.65	K	Joback Method
tf	236.04	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.50	J/mol×K	463.35	Joback Method
cpg	294.71	J/mol×K	493.73	Joback Method

cpg	307.32	J/mol×K	524.12	Joback Method
cpg	319.33	J/mol×K	554.50	Joback Method
cpg	330.78	J/mol×K	584.89	Joback Method
cpg	341.68	J/mol×K	615.27	Joback Method
cpg	352.05	J/mol×K	645.65	Joback Method
dvisc	0.0041736	Pa×s	236.04	Joback Method
dvisc	0.0018590	Pa×s	273.93	Joback Method
dvisc	0.0010078	Pa×s	311.81	Joback Method
dvisc	0.0006239	Pa×s	349.69	Joback Method
dvisc	0.0004242	Pa×s	387.58	Joback Method
dvisc	0.0003089	Pa×s	425.47	Joback Method
dvisc	0.0002369	Pa×s	463.35	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=C82456346&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
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume