5-Nonen-2-one

Other names: non-5-en-2-one
Inchi: InChI=1S/C9H16O/c1-3-4-5-6-7-8-9(2)10/h5-6H,3-4,7-8H2,1-2H3/b6-5+
InchiKey: RXFZCBZCGBDPDT-AATRIKPKSA-N
Formula: C9H16O
SMILES: CCCC=CCCC(C)=O
Mol. weight [g/mol]: 140.22
CAS: 27039-84-5

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
ripol	1435.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1437.00		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	341.68	J/mol×K	615.27	Joback Method
cpg	330.78	J/mol×K	584.89	Joback Method
cpg	319.33	J/mol×K	554.50	Joback Method
cpg	307.32	J/mol×K	524.12	Joback Method

cpg	294.71	J/mol×K	493.73	Joback Method
cpg	352.05	J/mol×K	645.65	Joback Method
dvisc	0.0002369	Pa×s	463.35	Joback Method
dvisc	0.0003089	Pa×s	425.47	Joback Method
dvisc	0.0004242	Pa×s	387.58	Joback Method
dvisc	0.0006239	Pa×s	349.69	Joback Method
dvisc	0.0010078	Pa×s	311.81	Joback Method
dvisc	0.0018590	Pa×s	273.93	Joback Method
dvisc	0.0041736	Pa×s	236.04	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27039845&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume