3,5-nonadien-2-one

Inchi: InChI=1S/C10H16O/c1-3-4-5-6-7-8-9-10(2)11/h6-9H,3-5H2,1-2H3/b7-6+,9-8+
InchiKey: KGVVLDOJDFWSCL-BLHCBFLLSA-N
Formula: C10H16O
SMILES: CCCCC=CC=CC(C)=O
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	64.84	kJ/mol	Joback Method
hf	-127.87	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	44.52	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1148.00		NIST Webbook
tb	490.39	K	Joback Method
tc	679.26	K	Joback Method
tf	242.23	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.35	J/mol×K	490.39	Joback Method
cpg	370.29	J/mol×K	647.79	Joback Method
cpg	359.21	J/mol×K	616.31	Joback Method
cpg	347.51	J/mol×K	584.83	Joback Method
cpg	335.16	J/mol×K	553.35	Joback Method
cpg	322.12	J/mol×K	521.87	Joback Method
cpg	380.80	J/mol×K	679.26	Joback Method
dvisc	0.0001895	Pa×s	490.39	Joback Method
dvisc	0.0002488	Pa×s	449.03	Joback Method

dvisc	0.0003453	Pa×s	407.67	Joback Method
dvisc	0.0005161	Pa×s	366.31	Joback Method
dvisc	0.0008544	Pa×s	324.95	Joback Method
dvisc	0.0016384	Pa×s	283.59	Joback Method
dvisc	0.0039242	Pa×s	242.23	Joback Method

Sources

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=R210689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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