3,5-Heptadien-2-one

Inchi: InChI=1S/C7H10O/c1-3-4-5-6-7(2)8/h3-6H,1-2H3/b4-3+,6-5+
InchiKey: SWGLACWOVFCDQS-VNKDHWASSA-N
Formula: C7H10O
SMILES: CC=CC=CC(C)=O
Mol. weight [g/mol]: 110.15
CAS: 3916-64-1

Physical Properties

Property code	Value	Unit	Source
gf	39.58	kJ/mol	Joback Method
hf	-65.95	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	37.84	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.708		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	1095.00		NIST Webbook
tb	421.75	K	Joback Method
tc	616.77	K	Joback Method
tf	208.42	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.52	J/mol×K	421.75	Joback Method
cpg	195.20	J/mol×K	454.25	Joback Method
cpg	205.27	J/mol×K	486.76	Joback Method
cpg	214.75	J/mol×K	519.26	Joback Method
cpg	223.68	J/mol×K	551.77	Joback Method
cpg	232.10	J/mol×K	584.27	Joback Method
cpg	240.03	J/mol×K	616.77	Joback Method
dvisc	0.0035142	Pa×s	208.42	Joback Method

dvisc	0.0015527	Pa×s	243.98	Joback Method
dvisc	0.0008444	Pa×s	279.53	Joback Method
dvisc	0.0005269	Pa×s	315.09	Joback Method
dvisc	0.0003618	Pa×s	350.64	Joback Method
dvisc	0.0002662	Pa×s	386.20	Joback Method
dvisc	0.0002063	Pa×s	421.75	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=C3916641&Units=SI

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