3,5-Octadien-2-one, isomer # 1

Inchi: InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h4-7H,3H2,1-2H3
InchiKey: LWRKMRFJEUFXIB-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CCC=CC=CC(C)=O
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
gf	48.00	kJ/mol	Joback Method
hf	-86.59	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
tb	444.63	K	Joback Method
tc	637.71	K	Joback Method
tf	219.69	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.73	J/mol×K	444.63	Joback Method
cpg	235.56	J/mol×K	476.81	Joback Method
cpg	246.73	J/mol×K	508.99	Joback Method
cpg	257.29	J/mol×K	541.17	Joback Method
cpg	267.25	J/mol×K	573.35	Joback Method
cpg	276.65	J/mol×K	605.53	Joback Method
cpg	285.54	J/mol×K	637.71	Joback Method
dvisc	0.0037387	Pa×s	219.69	Joback Method

dvisc	0.0016178	Pa×s	257.18	Joback Method
dvisc	0.0008664	Pa×s	294.67	Joback Method
dvisc	0.0005342	Pa×s	332.16	Joback Method
dvisc	0.0003633	Pa×s	369.65	Joback Method
dvisc	0.0002653	Pa×s	407.14	Joback Method
dvisc	0.0002043	Pa×s	444.63	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=R635439&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

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