(Z,Z)-octa-3,5-dien-2-one

Inchi: InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h4-7H,3H2,1-2H3/b5-4-,7-6-
InchiKey: LWRKMRFJEUFXIB-RZSVFLSASA-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
ripol	1520.00		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	276.65	J/mol×K	605.53	Joback Method
cpg	267.25	J/mol×K	573.35	Joback Method
cpg	257.29	J/mol×K	541.17	Joback Method
cpg	246.73	J/mol×K	508.99	Joback Method
cpg	235.56	J/mol×K	476.81	Joback Method
cpg	285.54	J/mol×K	637.71	Joback Method
dvisc	0.0002043	Pa×s	444.63	Joback Method
dvisc	0.0002653	Pa×s	407.14	Joback Method

dvisc	0.0003633	Pa×s	369.65	Joback Method
dvisc	0.0005342	Pa×s	332.16	Joback Method
dvisc	0.0008664	Pa×s	294.67	Joback Method
dvisc	0.0016178	Pa×s	257.18	Joback Method
dvisc	0.0037387	Pa×s	219.69	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=R315561&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume