

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

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	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
tb	444.63	K	Joback Method
tc	637.71	K	Joback Method
tf	219.69	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.73	J/molxK	444.63	Joback Method
cpg	276.65	J/molxK	605.53	Joback Method
cpg	267.25	J/molxK	573.35	Joback Method
cpg	257.29	J/molxK	541.17	Joback Method
cpg	246.73	J/molxK	508.99	Joback Method
cpg	235.56	J/molxK	476.81	Joback Method
cpg	285.54	J/molxK	637.71	Joback Method
dvisc	0.0002043	Paxs	444.63	Joback Method

dvisc	0.0002653	Paxs	407.14	Joback Method
dvisc	0.0003633	Paxs	369.65	Joback Method
dvisc	0.0005342	Paxs	332.16	Joback Method
dvisc	0.0008664	Paxs	294.67	Joback Method
dvisc	0.0016178	Paxs	257.18	Joback Method
dvisc	0.0037387	Paxs	219.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R635444&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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