

1,5-octadien-3-one

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C8H12O/c1-3-5-6-7-8(9)4-2/h4-6H,2-3,7H2,1H3/b6-5+

VWYBQOFZVSNDAW-AATRIKPKSA-N

C8H12O

C=CC(=O)CC=CCC

124.18

Physical Properties

Property code	Value	Unit	Source
gf	55.62	kJ/mol	Joback Method
hf	-78.38	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	984.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	988.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1358.00		NIST Webbook
tb	437.15	K	Joback Method
tc	625.01	K	Joback Method
tf	223.01	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.71	J/mol×K	437.15	Joback Method
cpg	275.88	J/mol×K	593.70	Joback Method

cpg	266.53	J/mol×K	562.39	Joback Method
cpg	256.66	J/mol×K	531.08	Joback Method
cpg	246.25	J/mol×K	499.77	Joback Method
cpg	235.28	J/mol×K	468.46	Joback Method
cpg	284.73	J/mol×K	625.01	Joback Method
dvisc	0.0002438	Pa×s	437.15	Joback Method
dvisc	0.0003125	Pa×s	401.46	Joback Method
dvisc	0.0004205	Pa×s	365.77	Joback Method
dvisc	0.0006033	Pa×s	330.08	Joback Method
dvisc	0.0009446	Pa×s	294.39	Joback Method
dvisc	0.0016740	Pa×s	258.70	Joback Method
dvisc	0.0035628	Pa×s	223.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R85237&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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