Oxepin, 2-methyl

Inchi: InChI=1S/C7H8O/c1-7-5-3-2-4-6-8-7/h2-6H,1H3
InchiKey: DMRHPVNNCCKLPE-UHFFFAOYSA-N
Formula: C7H8O
SMILES: CC1=CC=CC=CO1
Mol. weight [g/mol]: 108.14
CAS: 16479-77-9

Physical Properties

Property code	Value	Unit	Source
gf	22.25	kJ/mol	Joback Method
hf	-89.44	kJ/mol	Joback Method
hfus	13.81	kJ/mol	Joback Method
hvap	38.13	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.990		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	417.46	K	Joback Method
tc	638.17	K	Joback Method
tf	218.12	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.98	J/mol×K	417.46	Joback Method
cpg	174.94	J/mol×K	454.24	Joback Method
cpg	186.23	J/mol×K	491.03	Joback Method
cpg	196.86	J/mol×K	527.81	Joback Method
cpg	206.87	J/mol×K	564.60	Joback Method
cpg	216.25	J/mol×K	601.38	Joback Method
cpg	225.04	J/mol×K	638.17	Joback Method
dvisc	0.0056735	Pa×s	218.12	Joback Method
dvisc	0.0023660	Pa×s	251.34	Joback Method

dvisc	0.0012102	Pa×s	284.57	Joback Method
dvisc	0.0007122	Pa×s	317.79	Joback Method
dvisc	0.0004634	Pa×s	351.01	Joback Method
dvisc	0.0003247	Pa×s	384.24	Joback Method
dvisc	0.0002408	Pa×s	417.46	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=C16479779&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume