4-Methylhex-5-en-4-olide

Inchi: InChI=1S/C7H10O2/c1-3-7(2)5-4-6(8)9-7/h3H,1,4-5H2,2H3
InchiKey: QESPSAHXYXIGBG-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: C=CC1(C)CCC(=O)O1
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
gf	-81.75	kJ/mol	Joback Method
hf	-256.36	kJ/mol	Joback Method
hfus	7.73	kJ/mol	Joback Method
hvap	38.37	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.268		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
tb	466.53	K	Joback Method
tc	695.24	K	Joback Method
tf	296.48	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.01	J/mol×K	466.53	Joback Method
cpg	231.64	J/mol×K	504.65	Joback Method
cpg	244.35	J/mol×K	542.77	Joback Method
cpg	256.23	J/mol×K	580.88	Joback Method
cpg	267.38	J/mol×K	619.00	Joback Method
cpg	277.91	J/mol×K	657.12	Joback Method
cpg	287.91	J/mol×K	695.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R620838&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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