2-methoxy-2-buten-4-olide

Inchi: InChI=1S/C5H6O3/c1-7-4-2-3-8-5(4)6/h2H,3H2,1H3
InchiKey: LAPHJRDBCSBIPY-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: COC1=CCOC1=O
Mol. weight [g/mol]: 114.10

Physical Properties

Property code	Value	Unit	Source
gf	-257.90	kJ/mol	Joback Method
hf	-421.32	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	39.41	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	0.073		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
ripol	2043.00		NIST Webbook
ripol	2043.00		NIST Webbook
tb	455.08	K	Joback Method
tc	677.48	K	Joback Method
tf	291.55	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.87	J/mol×K	455.08	Joback Method
cpg	169.10	J/mol×K	492.15	Joback Method
cpg	178.06	J/mol×K	529.21	Joback Method
cpg	186.70	J/mol×K	566.28	Joback Method
cpg	195.02	J/mol×K	603.35	Joback Method
cpg	202.98	J/mol×K	640.42	Joback Method
cpg	210.56	J/mol×K	677.48	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=R319909&Units=SI

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