Propynal, dimethylacetal

Inchi: InChI=1S/C5H8O2/c1-4-5(6-2)7-3/h1,5H,2-3H3
InchiKey: OYSKRUJJSNSHLV-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: C#CC(OC)OC
Mol. weight [g/mol]: 100.12

Physical Properties

Property code	Value	Unit	Source
gf	1.85	kJ/mol	Joback Method
hf	-124.35	kJ/mol	Joback Method
hfus	10.53	kJ/mol	Joback Method
hvap	31.01	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.239		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	722.00		NIST Webbook
tb	348.32	K	Joback Method
tc	530.07	K	Joback Method
tf	222.54	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.64	J/mol×K	348.32	Joback Method
cpg	155.57	J/mol×K	378.61	Joback Method
cpg	162.37	J/mol×K	408.90	Joback Method
cpg	169.02	J/mol×K	439.19	Joback Method
cpg	175.52	J/mol×K	469.48	Joback Method
cpg	181.85	J/mol×K	499.77	Joback Method
cpg	188.03	J/mol×K	530.07	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=R512084&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume