Oxirane,cis-2,3-diethynyl-

Inchi: InChI=1S/C6H4O/c1-3-5-6(4-2)7-5/h1-2,5-6H/t5-,6+
InchiKey: ODHGCKRSONEWGS-OLQVQODUSA-N
Formula: C6H4O
SMILES: C#CC1OC1C#C
Mol. weight [g/mol]: 92.10
CAS: 40020-13-1

Physical Properties

Property code	Value	Unit	Source
gf	412.70	kJ/mol	Joback Method
hf	337.09	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	32.78	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-1.13		Crippen Method
logp	0.020		Crippen Method
mcvol	73.210	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	345.94	K	Joback Method
tc	554.24	K	Joback Method
tf	291.59	K	Joback Method
vc	0.273	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.84	J/mol×K	345.94	Joback Method
cpg	135.41	J/mol×K	380.66	Joback Method
cpg	143.35	J/mol×K	415.37	Joback Method
cpg	150.70	J/mol×K	450.09	Joback Method
cpg	157.49	J/mol×K	484.80	Joback Method
cpg	163.76	J/mol×K	519.52	Joback Method
cpg	169.56	J/mol×K	554.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40020131&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
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
ie:	Ionization energy
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