4-Ethyl-4-hydroxymethyl-2-methyl-delta^2-oxazol

Other names: 4-Ethyl-4-hydroxymethyl-2-methyl-delta
Inchi: InChI=1S/C7H13NO2/c1-3-7(4-9)5-10-6(2)8-7/h9H,3-5H2,1-2H3
InchiKey: CYBGFQUZJDXEBD-UHFFFAOYSA-N
Formula: C7H13NO2
SMILES: CCC1(CO)COC(C)=N1
Mol. weight [g/mol]: 143.18
CAS: 19383-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-46.71	kJ/mol	Joback Method
hf	-279.04	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	58.64	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.576		Crippen Method
mcvol	116.050	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	552.05	K	Joback Method
tc	756.83	K	Joback Method
tf	375.66	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.20	J/mol×K	552.05	Joback Method
cpg	312.53	J/mol×K	586.18	Joback Method
cpg	324.16	J/mol×K	620.31	Joback Method
cpg	335.17	J/mol×K	654.44	Joback Method
cpg	345.64	J/mol×K	688.57	Joback Method
cpg	355.64	J/mol×K	722.70	Joback Method
cpg	365.27	J/mol×K	756.83	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=C19383041&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume