2-Oxaspiro[3,4]octane

Inchi: InChI=1S/C7H12O/c1-2-4-7(3-1)5-6-8-7/h1-6H2
InchiKey: WQHMXROXEJWWGS-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C1CCC2(C1)CCO2
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	21.46	kJ/mol	Joback Method
hf	-150.95	kJ/mol	Joback Method
hfus	6.57	kJ/mol	Joback Method
hvap	35.01	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.719		Crippen Method
mcvol	93.640	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	950.00		NIST Webbook
tb	413.44	K	Joback Method
tc	636.13	K	Joback Method
tf	252.20	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.71	J/mol×K	413.44	Joback Method
cpg	206.71	J/mol×K	450.55	Joback Method
cpg	222.15	J/mol×K	487.67	Joback Method
cpg	236.20	J/mol×K	524.78	Joback Method
cpg	249.02	J/mol×K	561.90	Joback Method
cpg	260.77	J/mol×K	599.01	Joback Method
cpg	271.62	J/mol×K	636.13	Joback Method

Sources

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=R6552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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