

2-Oxaspiro[2,3]hexane

Inchi:	InChI=1S/C5H8O/c1-2-5(3-1)4-6-5/h1-4H2
InchiKey:	APUDJEBZDAGSQY-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C1CC2(C1)CO2
Mol. weight [g/mol]:	84.12

Physical Properties

Property code	Value	Unit	Source
gf	28.82	kJ/mol	Joback Method
hf	-97.35	kJ/mol	Joback Method
hfus	5.59	kJ/mol	Joback Method
hvap	30.22	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.939		Crippen Method
mcvol	65.460	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
rinpol	718.00		NIST Webbook
rinpol	718.00		NIST Webbook
tb	359.14	K	Joback Method
tc	567.19	K	Joback Method
tf	236.70	K	Joback Method
vc	0.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.15	J/mol×K	359.14	Joback Method
cpg	129.51	J/mol×K	393.81	Joback Method
cpg	141.44	J/mol×K	428.49	Joback Method
cpg	152.08	J/mol×K	463.16	Joback Method
cpg	161.57	J/mol×K	497.84	Joback Method
cpg	170.05	J/mol×K	532.51	Joback Method
cpg	177.66	J/mol×K	567.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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