2-Oxaspiro[3,3]heptane

Inchi: InChI=1S/C6H10O/c1-2-6(3-1)4-5-7-6/h1-5H2
InchiKey: KRFIYIXZGDGKNI-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C1CC2(C1)CCO2
Mol. weight [g/mol]: 98.14

Physical Properties

Property code	Value	Unit	Source
gf	25.14	kJ/mol	Joback Method
hf	-124.15	kJ/mol	Joback Method
hfus	6.08	kJ/mol	Joback Method
hvap	32.62	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.329		Crippen Method
mcvol	79.550	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
rinpol	842.00		NIST Webbook
tb	386.29	K	Joback Method
tc	602.01	K	Joback Method
tf	244.45	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.46	J/mol×K	386.29	Joback Method
cpg	166.64	J/mol×K	422.24	Joback Method
cpg	180.32	J/mol×K	458.20	Joback Method
cpg	192.65	J/mol×K	494.15	Joback Method
cpg	203.80	J/mol×K	530.11	Joback Method
cpg	213.91	J/mol×K	566.06	Joback Method
cpg	223.13	J/mol×K	602.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6549&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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