1,7-Dioxaspiro[5.5]undecane

Inchi: InChI=1S/C9H16O2/c1-3-7-10-9(5-1)6-2-4-8-11-9/h1-8H2
InchiKey: GBBVHDGKDQAEOT-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C1CCC2(CCCCO2)OC1
Mol. weight [g/mol]: 156.22
CAS: 180-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-84.12	kJ/mol	Joback Method
hf	-342.71	kJ/mol	Joback Method
hfus	13.42	kJ/mol	Joback Method
hvap	44.49	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.084		Crippen Method
mcvol	127.690	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	498.96	K	Joback Method
tc	740.96	K	Joback Method
tf	290.75	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.40	J/mol×K	498.96	Joback Method
cpg	327.99	J/mol×K	539.29	Joback Method
cpg	346.95	J/mol×K	579.63	Joback Method
cpg	364.46	J/mol×K	619.96	Joback Method
cpg	380.71	J/mol×K	660.30	Joback Method
cpg	395.86	J/mol×K	700.63	Joback Method
cpg	410.09	J/mol×K	740.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	466.20	K	100.00	NIST Webbook

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=C180847&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume