theaspirane

Other names:	2,6,10,10-Tetramethyl-1-oxa-spiro[4.5]-dec-6-ene
	Theaspirane (Isomer 2)
	Theaspirane (Isomer 1)
Inchi:	InChI=1S/C13H22O/c1-10-6-5-8-12(3,4)13(10)9-7-11(2)14-13/h6,11H,5,7-9H2,1-4H3
InchiKey:	GYUZHTWCNKINPY-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	CC1=CCCC(C)(C)C12CCC(C)O2
Mol. weight [g/mol]:	194.31
CAS:	36431-72-8

Physical Properties

Property code	Value	Unit	Source
gf	47.20	kJ/mol	Joback Method
hf	-266.24	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.690		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1298.10		NIST Webbook
rinpol	1302.50		NIST Webbook
rinpol	1305.20		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1302.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1533.00		NIST Webbook

ripol	1496.00		NIST Webbook
tb	554.30	K	Joback Method
tc	785.37	K	Joback Method
tf	341.48	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.24	J/mol×K	554.30	Joback Method
cpg	473.01	J/mol×K	592.81	Joback Method
cpg	493.29	J/mol×K	631.32	Joback Method
cpg	512.34	J/mol×K	669.83	Joback Method
cpg	530.43	J/mol×K	708.35	Joback Method
cpg	547.81	J/mol×K	746.86	Joback Method
cpg	564.75	J/mol×K	785.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36431728&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume