9-(4-Methylpentene-3-yl) spiro[5.5]undecene-8-one-1

Inchi: InChI=1S/C17H26O/c1-14(2)6-5-7-15-9-12-17(13-10-15)11-4-3-8-16(17)18/h6,9H,3-5,7-8

InchiKey: GQKQQSMFSHMOKY-UHFFFAOYSA-N

Formula: C17H26O

SMILES: CC(C)=CCCC1=CCC2(CCCCC2=O)CC1

Mol. weight [g/mol]: 246.39

Physical Properties

Property code	Value	Unit	Source
gf	124.89	kJ/mol	Joback Method
hf	-227.79	kJ/mol	Joback Method
hfus	17.42	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.973		Crippen Method
mcvol	221.640	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1953.20		NIST Webbook
rinpol	1967.70		NIST Webbook
rinpol	1953.20		NIST Webbook
ripol	2490.10		NIST Webbook
ripol	2506.20		NIST Webbook
ripol	2490.10		NIST Webbook
tb	704.10	K	Joback Method
tc	944.31	K	Joback Method
tf	390.23	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.49	J/mol×K	704.10	Joback Method
cpg	674.36	J/mol×K	744.13	Joback Method
cpg	696.00	J/mol×K	784.17	Joback Method
cpg	716.60	J/mol×K	824.20	Joback Method

cpg	736.34	J/mol×K	864.24	Joback Method
cpg	755.40	J/mol×K	904.27	Joback Method
cpg	773.98	J/mol×K	944.31	Joback Method

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=R261033&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
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