8-(4-Methylpentene-3-yl) spiro[4.5]decene-7-one-1

Inchi: InChI=1S/C16H24O/c1-13(2)5-3-6-14-8-11-16(12-9-14)10-4-7-15(16)17/h5,8H,3-4,6-7,9-

InchiKey: SWIZJNCHDUBHJE-UHFFFAOYSA-N

Formula: C16H24O

SMILES: CC(C)=CCCC1=CCC2(CCCC2=O)CC1

Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
gf	128.57	kJ/mol	Joback Method
hf	-200.99	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	56.12	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.583		Crippen Method
mcvol	207.550	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1853.20		NIST Webbook
ripol	2374.40		NIST Webbook
ripol	2387.30		NIST Webbook
tb	676.95	K	Joback Method
tc	914.56	K	Joback Method
tf	382.48	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.65	J/mol×K	676.95	Joback Method
cpg	614.31	J/mol×K	716.55	Joback Method
cpg	634.79	J/mol×K	756.15	Joback Method
cpg	654.27	J/mol×K	795.76	Joback Method
cpg	672.95	J/mol×K	835.36	Joback Method
cpg	690.99	J/mol×K	874.96	Joback Method

cpg	708.60	J/mol×K	914.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R261013&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

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