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

Inchi: InChI=1S/C16H24O/c1-13(2)6-3-7-14-8-4-10-16(12-14)11-5-9-15(16)17/h6,8H,3-5,7,9-12

InchiKey: UHNRJWOMCSGFRV-UHFFFAOYSA-N

Formula: C16H24O

SMILES: CC(C)=CCCC1=CCCC2(CCCC2=O)C1

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	1826.50		NIST Webbook
rinpol	1834.60		NIST Webbook
rinpol	1826.50		NIST Webbook
ripol	2356.10		NIST Webbook
ripol	2344.90		NIST Webbook
ripol	2344.90		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

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=R261008&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