

4-(2,2,6-Trimethyl-1-oxaspiro[4.4]non-6-en-3-yl)-b

Other names:	Taylofuran
Inchi:	InChI=1S/C15H24O2/c1-11-6-5-9-15(11)10-13(8-7-12(2)16)14(3,4)17-15/h6,13H,5,7-10H
InchiKey:	WIQUMZFHDBZVSM-UKRRQHHQSA-N
Formula:	C15H24O2
SMILES:	CC(=O)CCC1CC2(CCC=C2C)OC1(C)C
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-52.78	kJ/mol	Joback Method
hf	-413.94	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	58.92	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.650		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	649.66	K	Joback Method
tc	871.67	K	Joback Method
tf	417.47	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.28	J/mol×K	649.66	Joback Method
cpg	598.94	J/mol×K	686.66	Joback Method
cpg	617.70	J/mol×K	723.66	Joback Method
cpg	635.79	J/mol×K	760.67	Joback Method
cpg	653.47	J/mol×K	797.67	Joback Method
cpg	670.97	J/mol×K	834.67	Joback Method
cpg	688.55	J/mol×K	871.67	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=R407799&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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