

Helifolen-14-yl methyl ether

Inchi:	InChI=1S/C16H26O/c1-12-5-6-13-14(2,3)15(11-17-4)7-9-16(12,13)10-8-15/h7,9,12-13H,
InchiKey:	QPJVWPGTAOGEF-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	COCC12C=CC3(CC1)C(C)CCC3C2(C)C
Mol. weight [g/mol]:	234.38

Physical Properties

Property code	Value	Unit	Source
gf	134.96	kJ/mol	Joback Method
hf	-236.89	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.042		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinqol	1613.00		NIST Webbook
ripol	1940.00		NIST Webbook
tb	607.20	K	Joback Method
tc	833.38	K	Joback Method
tf	403.07	K	Joback Method
vc	0.782	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.75	J/mol×K	607.20	Joback Method
cpg	606.34	J/mol×K	644.90	Joback Method
cpg	627.67	J/mol×K	682.59	Joback Method
cpg	648.10	J/mol×K	720.29	Joback Method
cpg	668.04	J/mol×K	757.99	Joback Method
cpg	687.87	J/mol×K	795.69	Joback Method
cpg	707.98	J/mol×K	833.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R236250&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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