8,9-Dehydrothymol methyl ether

Inchi: InChI=1S/C11H14O/c1-8(2)10-6-5-9(3)7-11(10)12-4/h5-7H,1H2,2-4H3
InchiKey: LDQHURFLDDRWGZ-UHFFFAOYSA-N
Formula: C11H14O
SMILES: C=C(C)c1ccc(C)cc1OC
Mol. weight [g/mol]: 162.23
CAS: 39701-08-1

Physical Properties

Property code	Value	Unit	Source
gf	109.18	kJ/mol	Joback Method
hf	-73.36	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	45.50	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.037		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1247.20		NIST Webbook
tb	506.70	K	Joback Method
tc	717.72	K	Joback Method
tf	271.70	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.07	J/mol×K	506.70	Joback Method
cpg	322.57	J/mol×K	541.87	Joback Method
cpg	336.36	J/mol×K	577.04	Joback Method
cpg	349.45	J/mol×K	612.21	Joback Method
cpg	361.85	J/mol×K	647.38	Joback Method
cpg	373.59	J/mol×K	682.55	Joback Method
cpg	384.68	J/mol×K	717.72	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=C39701081&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume