8,9-Dehydrothymol

Inchi: InChI=1S/C10H12O/c1-7(2)9-5-4-8(3)6-10(9)11/h4-6,11H,1H2,2-3H3
InchiKey: IHWFPRKZRRGTTI-UHFFFAOYSA-N
Formula: C10H12O
SMILES: C=C(C)c1ccc(C)cc1O
Mol. weight [g/mol]: 148.20
CAS: 18612-99-2

Physical Properties

Property code	Value	Unit	Source
gf	60.77	kJ/mol	Joback Method
hf	-86.34	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.734		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1221.10		NIST Webbook
rinpol	1221.10		NIST Webbook
ripol	2006.00		NIST Webbook
tb	537.04	K	Joback Method
tc	765.73	K	Joback Method
tf	337.40	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.22	J/mol×K	537.04	Joback Method
cpg	305.19	J/mol×K	575.16	Joback Method
cpg	317.23	J/mol×K	613.27	Joback Method
cpg	328.44	J/mol×K	651.39	Joback Method
cpg	338.90	J/mol×K	689.50	Joback Method
cpg	348.71	J/mol×K	727.62	Joback Method

cpg	357.95	J/mol×K	765.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18612992&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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