8,9-Dehydrothymol isobutyrate

Inchi: InChI=1S/C14H18O2/c1-9(2)12-7-6-11(5)13(8-12)16-14(15)10(3)4/h6-8,10H,1H2,2-5H3
InchiKey: KICUJBIVPALHON-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: C=C(C)c1ccc(C)c(OC(=O)C(C)C)c1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	3.08	kJ/mol	Joback Method
hf	-253.14	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.590		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	628.77	K	Joback Method
tc	841.84	K	Joback Method
tf	340.44	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.75	J/mol×K	628.77	Joback Method
cpg	487.67	J/mol×K	664.28	Joback Method
cpg	502.68	J/mol×K	699.79	Joback Method
cpg	516.80	J/mol×K	735.31	Joback Method
cpg	530.05	J/mol×K	770.82	Joback Method
cpg	542.46	J/mol×K	806.33	Joback Method

cpg	554.04	J/mol×K	841.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204372&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume