

8,9-Dehydrothymyl methacrylate

Inchi:	InChI=1S/C14H16O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h6-8H,1,3H2,2,4-5H3
InchiKey:	GYZZSDPJKDCFRU-UHFFFAOYSA-N
Formula:	C14H16O2
SMILES:	<chem>C=C(C)C(=O)Oc1cc(C)ccc1C(=C)C</chem>
Mol. weight [g/mol]:	216.28

Physical Properties

Property code	Value	Unit	Source
gf	84.81	kJ/mol	Joback Method
hf	-132.22	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.510		Crippen Method
mvol	183.200	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
ripol	1479.00		NIST Webbook
ripol	2116.00		NIST Webbook
tb	625.77	K	Joback Method
tc	842.36	K	Joback Method
tf	339.72	K	Joback Method
vc	0.700	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.29	J/molxK	625.77	Joback Method
cpg	464.47	J/molxK	661.87	Joback Method
cpg	478.75	J/molxK	697.97	Joback Method
cpg	492.16	J/molxK	734.07	Joback Method
cpg	504.73	J/molxK	770.16	Joback Method
cpg	516.48	J/molxK	806.26	Joback Method
cpg	527.45	J/molxK	842.36	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=R518200&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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