

8,9-Dehydrothymyl isovalerate

Inchi:	InChI=1S/C15H20O2/c1-10(2)8-15(16)17-14-9-12(5)6-7-13(14)11(3)4/h6-7,9-10H,3,8H2
InchiKey:	DISRRWDKWSKYMA-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	<chem>C=C(C)c1ccc(C)cc1OC(=O)CC(C)C</chem>
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
gf	11.50	kJ/mol	Joback Method
hf	-273.78	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.980		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
ripol	1548.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
tb	651.65	K	Joback Method
tc	861.36	K	Joback Method
tf	351.71	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.30	J/mol×K	651.65	Joback Method
cpg	539.74	J/mol×K	686.60	Joback Method
cpg	555.22	J/mol×K	721.55	Joback Method
cpg	569.79	J/mol×K	756.51	Joback Method

cpg	583.47	J/mol×K	791.46	Joback Method
cpg	596.27	J/mol×K	826.41	Joback Method
cpg	608.23	J/mol×K	861.36	Joback Method

Sources

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=R417206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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