

Thymyl angelate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H20O2/c1-6-12(5)15(16)17-14-9-11(4)7-8-13(14)10(2)3/h6-10H,1-5H3/b12

UUEIVUJSJLKAAM-WUXMJOGZSA-N

C15H20O2

CC=C(C)C(=O)Oc1cc(C)ccc1C(C)C

232.32

101162-18-9

Physical Properties

Property code	Value	Unit	Source
gf	3.88	kJ/mol	Joback Method
hf	-281.99	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	61.39	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.990		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1664.20		NIST Webbook
rinpol	1664.20		NIST Webbook
rinpol	1582.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
tb	659.13	K	Joback Method
tc	873.07	K	Joback Method
tf	348.39	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.22	J/mol×K	659.13	Joback Method
cpg	540.72	J/mol×K	694.79	Joback Method
cpg	556.26	J/mol×K	730.44	Joback Method

cpg	570.85	J/mol×K	766.10	Joback Method
cpg	584.54	J/mol×K	801.76	Joback Method
cpg	597.36	J/mol×K	837.42	Joback Method
cpg	609.35	J/mol×K	873.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101162189&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

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