

Helifolen-12-oic acid (anti-syn-syn)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H22O2/c1-10-4-5-11-14(3,12(16)17)13(2)6-8-15(10,11)9-7-13/h6,8,10-11H

CFOAFRDJZWKHED-UHFFFAOYSA-N

C15H22O2

CC1CCC2C13C=CC(C)(CC3)C2(C)C(=O)O

234.33

Physical Properties

Property code	Value	Unit	Source
gf	-34.20	kJ/mol	Joback Method
hf	-348.84	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	707.95	K	Joback Method
tc	929.41	K	Joback Method
tf	480.32	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.53	J/mol×K	707.95	Joback Method
cpg	610.11	J/mol×K	744.86	Joback Method
cpg	627.53	J/mol×K	781.77	Joback Method
cpg	645.18	J/mol×K	818.68	Joback Method
cpg	663.42	J/mol×K	855.59	Joback Method
cpg	682.63	J/mol×K	892.50	Joback Method
cpg	703.20	J/mol×K	929.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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