MEGASTIGMATRIENONE

Inchi: InChI=1S/C13H18O/c1-5-6-7-12-10(2)8-11(14)9-13(12,3)4/h5-8,12H,1,9H2,2-4H3/b7-6+
InchiKey: YKVWPZJHENXDAJ-VOTSOKGWSA-N
Formula: C13H18O
SMILES: C=C/C=C/C1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 190.29

Physical Properties

Property code	Value	Unit	Source
hfus	15.30	kJ/mol	Joback Method
logp	3.290		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
rinpol	1473.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.27	J/mol×K	584.76	Joback Method
cpg	447.05	J/mol×K	622.87	Joback Method
cpg	464.77	J/mol×K	660.98	Joback Method
cpg	481.55	J/mol×K	699.08	Joback Method
cpg	497.51	J/mol×K	737.19	Joback Method
cpg	512.77	J/mol×K	775.30	Joback Method
cpg	527.45	J/mol×K	813.41	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38818552&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices