Rotundone

Inchi: InChI=1S/C15H22O/c1-9(2)12-6-5-10(3)15-13(8-12)11(4)7-14(15)16/h10-12H,1,5-8H2,2-
InchiKey: NUWMTBMCSQWPDG-SDDRHHMPSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C)C2=C(C1)C(C)CC2=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	20.91	kJ/mol	Joback Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1712.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1703.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.27	J/mol×K	641.99	Joback Method
cpg	565.40	J/mol×K	680.30	Joback Method
cpg	586.17	J/mol×K	718.60	Joback Method
cpg	605.60	J/mol×K	756.91	Joback Method
cpg	623.72	J/mol×K	795.21	Joback Method
cpg	640.55	J/mol×K	833.52	Joback Method
cpg	656.12	J/mol×K	871.82	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R613073&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):	
Cheméo Relay (1.0, beta):	

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