Cyclocolorenone

Inchi: InChI=1S/C15H22O/c1-8-5-6-11-14(15(11,3)4)13-9(2)12(16)7-10(8)13/h8,10-11,14H,5-7
InchiKey: ZEEUIOBUKGZKPS-LJCHNNMDSA-N
Formula: C15H22O
SMILES: CC1=C2C(CC1=O)C(C)CCC1C2C1(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	20.61	kJ/mol	Joback Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
rinpol	1745.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1745.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/mol×K	639.20	Joback Method
cpg	567.48	J/mol×K	677.62	Joback Method
cpg	587.88	J/mol×K	716.04	Joback Method
cpg	607.27	J/mol×K	754.46	Joback Method
cpg	625.82	J/mol×K	792.88	Joback Method
cpg	643.70	J/mol×K	831.30	Joback Method
cpg	661.06	J/mol×K	869.72	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R604861&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

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