cis-«beta»-Damascenone

Inchi: InChI=1S/C13H18O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-8H,9H2,1-4H3/b7-5-
InchiKey: POIARNZEYGURDG-ALCCZGGFSA-N
Formula: C13H18O
SMILES: CC=CC(=O)C1=C(C)C=CCC1(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
hfus	18.43	kJ/mol	Joback Method
logp	3.434		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.12	J/mol×K	582.94	Joback Method
cpg	433.84	J/mol×K	619.80	Joback Method
cpg	449.57	J/mol×K	656.67	Joback Method
cpg	464.42	J/mol×K	693.53	Joback Method
cpg	478.54	J/mol×K	730.40	Joback Method
cpg	492.06	J/mol×K	767.26	Joback Method
cpg	505.11	J/mol×K	804.13	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=R630890&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