«alpha»-Damascenone

Inchi: InChI=1S/C13H18O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-9,12H,1-4H3/b7-5+
InchiKey: JGBBQKAJVHEQJM-FNORWQNLSA-N
Formula: C13H18O
SMILES: CC=CC(=O)C1C(C)=CC=CC1(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
hfus	19.89	kJ/mol	Joback Method
logp	3.290		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1813.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.67	J/mol×K	573.29	Joback Method
cpg	436.18	J/mol×K	609.98	Joback Method
cpg	452.61	J/mol×K	646.67	Joback Method
cpg	468.10	J/mol×K	683.35	Joback Method
cpg	482.77	J/mol×K	720.04	Joback Method
cpg	496.77	J/mol×K	756.73	Joback Method
cpg	510.21	J/mol×K	793.42	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R613464&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
ripol:	Polar retention indices