(E)-«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-FNORWQNLSA-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	1385.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1390.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1815.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R598835&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
ripol:	Polar retention indices