trans-«beta»-Damascone

Inchi: InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5,7H,6,8-9H2,1-4H3/b7-5+
InchiKey: BGTBFNDXYDYBEY-FNORWQNLSA-N
Formula: C13H20O
SMILES: CC=CC(=O)C1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	17.21	kJ/mol	Joback Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1441.00		NIST Webbook
rinpol	1414.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.25	J/mol×K	583.78	Joback Method
cpg	455.12	J/mol×K	620.30	Joback Method
cpg	471.95	J/mol×K	656.81	Joback Method
cpg	487.87	J/mol×K	693.33	Joback Method
cpg	503.02	J/mol×K	729.85	Joback Method
cpg	517.51	J/mol×K	766.36	Joback Method
cpg	531.49	J/mol×K	802.88	Joback Method

Sources

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):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R571954&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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