(S)-2,6,6-Trimethyl-2-((2S,5S)-5-methyl-5-vinyltetra

Inchi: InChI=1S/C15H22O3/c1-6-14(4)10-8-12(17-14)15(5)11(16)7-9-13(2,3)18-15/h6-7,9,12H,
InchiKey: YDGSUVJUYWCJCE-SNPRPXQTSA-N
Formula: C15H22O3
SMILES: C=CC1(C)CCC(C2(C)OC(C)(C)C=CC2=O)O1
Mol. weight [g/mol]: 250.33
CAS: 115403-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-72.50	kJ/mol	Joback Method
hf	-451.58	kJ/mol	Joback Method
hfus	19.03	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.803		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1566.20		NIST Webbook
tb	686.37	K	Joback Method
tc	938.78	K	Joback Method
tf	460.67	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.71	J/mol×K	686.37	Joback Method
cpg	627.81	J/mol×K	728.44	Joback Method
cpg	649.33	J/mol×K	770.51	Joback Method
cpg	670.71	J/mol×K	812.57	Joback Method
cpg	692.36	J/mol×K	854.64	Joback Method
cpg	714.72	J/mol×K	896.71	Joback Method
cpg	738.19	J/mol×K	938.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115403991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume