(1R,3aR,5aR,9aS)-1,4,4,7-Tetramethyl-1,2,3,3a,4,5a

Inchi: InChI=1S/C15H24O/c1-10-7-8-15-11(2)5-6-12(15)14(3,4)16-13(15)9-10/h9,11-13H,5-8H2
InchiKey: JGKMDLIITSKWAD-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1=CC2OC(C)(C)C3CCC(C)C23CC1
Mol. weight [g/mol]: 220.35
CAS: 104188-25-2

Physical Properties

Property code	Value	Unit	Source
gf	129.18	kJ/mol	Joback Method
hf	-248.90	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1544.40		NIST Webbook
rinpol	1544.40		NIST Webbook
tb	597.86	K	Joback Method
tc	828.69	K	Joback Method
tf	381.24	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.74	J/mol×K	597.86	Joback Method
cpg	563.58	J/mol×K	636.33	Joback Method
cpg	584.99	J/mol×K	674.80	Joback Method
cpg	605.27	J/mol×K	713.28	Joback Method
cpg	624.73	J/mol×K	751.75	Joback Method
cpg	643.66	J/mol×K	790.22	Joback Method
cpg	662.37	J/mol×K	828.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C104188252&Units=SI

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