(1S,3aS,4S,7R,8aS)-1,4,9,9-Tetramethyldecahydro

Inchi: InChI=1S/C15H26O2/c1-10-5-8-15(16)12(10)9-11-6-7-14(15,4)17-13(11,2)3/h10-12,16H
InchiKey: OSXGCNJUBCSZET-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC1CCC2(O)C1CC1CCC2(C)OC1(C)C
Mol. weight [g/mol]: 238.37
CAS: 94388-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-41.17	kJ/mol	Joback Method
hf	-452.54	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	66.05	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.131		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1673.60		NIST Webbook
tb	681.47	K	Joback Method
tc	899.32	K	Joback Method
tf	448.44	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.75	J/mol×K	681.47	Joback Method
cpg	653.00	J/mol×K	717.78	Joback Method
cpg	672.69	J/mol×K	754.09	Joback Method
cpg	692.18	J/mol×K	790.40	Joback Method
cpg	711.81	J/mol×K	826.71	Joback Method
cpg	731.91	J/mol×K	863.02	Joback Method
cpg	752.82	J/mol×K	899.32	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=C94388633&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