(3aS,4R,7R)-1,4,9,9-Tetramethyl-5,6,7,8-tetrahydro

Inchi: InChI=1S/C15H22/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h7-8,11-12H,5-6,9H2
InchiKey: DPHLFUXQEZYZAP-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC1=C2CC3CCC(C)C2(C=C1)C3(C)C
Mol. weight [g/mol]: 202.34
CAS: 50430-14-3

Physical Properties

Property code	Value	Unit	Source
gf	255.44	kJ/mol	Joback Method
hf	-44.09	kJ/mol	Joback Method
hfus	14.95	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1369.40		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	575.45	K	Joback Method
tc	804.27	K	Joback Method
tf	375.71	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.52	J/mol×K	575.45	Joback Method
cpg	504.45	J/mol×K	613.59	Joback Method
cpg	523.95	J/mol×K	651.72	Joback Method
cpg	542.31	J/mol×K	689.86	Joback Method
cpg	559.86	J/mol×K	728.00	Joback Method

cpg	576.90	J/mol×K	766.14	Joback Method
cpg	593.73	J/mol×K	804.27	Joback Method

Sources

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=C50430143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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