(1R,3aS,4R,7R,8aR)-1,4-Dimethyl-1,2,3,3a,4,7,8,8a-

Inchi: InChI=1S/C14H22/c1-10-3-4-13-12(10)9-11-5-7-14(13,2)8-6-11/h5,7,10-13H,3-4,6,8-9H2
InchiKey: CFEBVBFXLFAFIO-UHFFFAOYSA-N
Formula: C14H22
SMILES: CC1CCC2C1CC1C=CC2(C)CC1
Mol. weight [g/mol]: 190.32
CAS: 394217-22-2

Physical Properties

Property code	Value	Unit	Source
gf	222.00	kJ/mol	Joback Method
hf	-100.03	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	45.54	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.025		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1433.50		NIST Webbook
tb	542.81	K	Joback Method
tc	770.33	K	Joback Method
tf	306.98	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.06	J/mol×K	542.81	Joback Method
cpg	477.46	J/mol×K	580.73	Joback Method
cpg	500.11	J/mol×K	618.65	Joback Method
cpg	521.22	J/mol×K	656.57	Joback Method
cpg	540.98	J/mol×K	694.49	Joback Method
cpg	559.60	J/mol×K	732.41	Joback Method
cpg	577.27	J/mol×K	770.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394217222&Units=SI
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

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