(2S,3aR,3bR,4R,7aS)-7,7,8,8-Tetramethyloctahydr

Inchi: InChI=1S/C15H24O/c1-12(2)6-5-11(16)15-10-7-9(13(15,3)4)8-14(10,12)15/h9-11,16H,5-
InchiKey: URRFLKHHGNPGCX-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1(C)CCC(O)C23C4CC(CC412)C3(C)C
Mol. weight [g/mol]: 220.35
CAS: 74841-81-9

Physical Properties

Property code	Value	Unit	Source
gf	148.61	kJ/mol	Joback Method
hf	-207.86	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.220		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1518.70		NIST Webbook
rinpol	1518.70		NIST Webbook
tb	644.42	K	Joback Method
tc	859.30	K	Joback Method
tf	477.79	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.32	J/mol×K	644.42	Joback Method
cpg	589.13	J/mol×K	680.23	Joback Method
cpg	606.38	J/mol×K	716.05	Joback Method
cpg	623.54	J/mol×K	751.86	Joback Method
cpg	641.07	J/mol×K	787.68	Joback Method
cpg	659.45	J/mol×K	823.49	Joback Method
cpg	679.14	J/mol×K	859.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74841819&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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