(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-Trimethyldecahyd

Other names: Ishwaran
Ishwarane
(-)-Ishwarane
1,2a-Methano-2aH-cyclopropa[b]naphthalene, decahydro-1,6,6a-trimethyl-, [1R-(1«alpha»,1a«beta»,2a«alpha»,6«beta»,6a«beta»,7a«alpha»)]-

Inchi: InChI=1S/C15H24/c1-10-5-4-6-15-8-12-11(7-14(10,15)3)13(12,2)9-15/h10-12H,4-9H2,1-3

InchiKey: XGEWXQPYPMTSBD-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC1CCCC23CC4C(CC12C)C4(C)C3

Mol. weight [g/mol]: 204.35

CAS: 26620-70-2

Physical Properties

Property code	Value	Unit	Source
gf	286.53	kJ/mol	Joback Method
hf	-56.69	kJ/mol	Joback Method
hfus	10.39	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.249		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1458.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1644.00		NIST Webbook
tb	560.94	K	Joback Method
tc	793.13	K	Joback Method
tf	393.79	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.93	J/mol×K	560.94	Joback Method
cpg	528.33	J/mol×K	599.64	Joback Method
cpg	549.82	J/mol×K	638.34	Joback Method
cpg	569.89	J/mol×K	677.04	Joback Method
cpg	589.02	J/mol×K	715.74	Joback Method
cpg	607.70	J/mol×K	754.43	Joback Method
cpg	626.43	J/mol×K	793.13	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=C26620702&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume