Herbertene

Inchi: InChI=1S/C15H22/c1-12-7-5-8-13(11-12)15(4)10-6-9-14(15,2)3/h5,7-8,11H,6,9-10H2,1-4
InchiKey: BBZBREYBGRYINI-HNNXBMFYSA-N
Formula: C15H22
SMILES: Cc1cccc(C2(C)CCCC2(C)C)c1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	196.06	kJ/mol	Joback Method
hf	-57.25	kJ/mol	Joback Method
hfus	10.67	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.463		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	585.35	K	Joback Method
tc	824.05	K	Joback Method
tf	352.21	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.48	J/mol×K	585.35	Joback Method
cpg	501.95	J/mol×K	625.13	Joback Method
cpg	522.02	J/mol×K	664.92	Joback Method
cpg	541.00	J/mol×K	704.70	Joback Method
cpg	559.17	J/mol×K	744.48	Joback Method
cpg	576.82	J/mol×K	784.27	Joback Method
cpg	594.26	J/mol×K	824.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R639991&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