(+)-Isobicyclogermacrene

Inchi: InChI=1S/C15H24/c1-11-6-5-7-12(2)10-14-13(9-8-11)15(14,3)4/h8,10,13-14H,5-7,9H2,1-
InchiKey: XQWHVETYKWCCGI-MHTRXRHISA-N
Formula: C15H24
SMILES: CC1=CCC2C(C=C(C)CCC1)C2(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	163.88	kJ/mol	Joback Method
hf	-150.61	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	581.28	K	Joback Method
tc	808.29	K	Joback Method
tf	323.31	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/mol×K	581.28	Joback Method
cpg	526.59	J/mol×K	619.11	Joback Method
cpg	548.47	J/mol×K	656.95	Joback Method
cpg	569.08	J/mol×K	694.78	Joback Method
cpg	588.58	J/mol×K	732.62	Joback Method
cpg	607.10	J/mol×K	770.45	Joback Method
cpg	624.78	J/mol×K	808.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434578&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