Isobicyclogermacrenal

Inchi: InChI=1S/C15H22O/c1-11-5-4-6-12(2)9-14-13(8-7-11)15(14,3)10-16/h5,9-10,13-14H,4,6-
InchiKey: PLERVCQIUZNKMR-FYJMDNOOSA-N
Formula: C15H22O
SMILES: CC1=CC2C(CCC(C)=CCC1)C2(C)C=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	64.36	kJ/mol	Joback Method
hf	-236.19	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	56.84	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	629.94	K	Joback Method
tc	858.86	K	Joback Method
tf	365.31	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.57	J/mol×K	629.94	Joback Method
cpg	551.52	J/mol×K	668.09	Joback Method
cpg	571.23	J/mol×K	706.25	Joback Method
cpg	589.86	J/mol×K	744.40	Joback Method
cpg	607.55	J/mol×K	782.55	Joback Method
cpg	624.44	J/mol×K	820.71	Joback Method
cpg	640.69	J/mol×K	858.86	Joback Method

Sources

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=R617595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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