Hexahydrogermacrone-c

Inchi: InChI=1S/C15H28O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h11-14H,5-10H2,1-4H3
InchiKey: IVZVLIBJTFLRJR-UHFFFAOYSA-N
Formula: C15H28O
SMILES: CC1CCCC(C)CC(=O)C(C(C)C)CC1
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-88.98	kJ/mol	Joback Method
hf	-506.91	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.454		Crippen Method
mcvol	212.920	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1967.00		NIST Webbook
tb	637.27	K	Joback Method
tc	866.15	K	Joback Method
tf	296.85	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.85	J/mol×K	637.27	Joback Method
cpg	637.95	J/mol×K	675.42	Joback Method
cpg	663.42	J/mol×K	713.56	Joback Method
cpg	687.20	J/mol×K	751.71	Joback Method
cpg	709.27	J/mol×K	789.86	Joback Method
cpg	729.58	J/mol×K	828.00	Joback Method

cpg	748.10	J/mol×K	866.15	Joback Method

Sources

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=R306582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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