2(3H)-Benzofuranone, hexahydro-4,4,7a-trimethyl-

Other names: Tetrahydroactinidiolide
Hexahydro-4,4,7a-trimethyl-2-benzofuranone
Inchi: InChI=1S/C11H18O2/c1-10(2)5-4-6-11(3)8(10)7-9(12)13-11/h8H,4-7H2,1-3H3
InchiKey: IGSYVKHPYSDDQD-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CC1(C)CCCC2(C)OC(=O)CC12
Mol. weight [g/mol]: 182.26
CAS: 16778-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-100.46	kJ/mol	Joback Method
hf	-402.81	kJ/mol	Joback Method
hfus	10.18	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.518		Crippen Method
mcvol	151.570	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
ripol	2305.00		NIST Webbook
tb	567.95	K	Joback Method
tc	811.06	K	Joback Method
tf	377.40	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.29	J/mol×K	567.95	Joback Method
cpg	425.29	J/mol×K	608.47	Joback Method
cpg	443.99	J/mol×K	648.99	Joback Method
cpg	461.66	J/mol×K	689.51	Joback Method
cpg	478.57	J/mol×K	730.03	Joback Method
cpg	494.98	J/mol×K	770.55	Joback Method

cpg	511.17	J/mol×K	811.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16778271&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume