2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-

Other names: (2,6,6-Trimethyl-2-hydroxycyclohexylidene)acetic acid lactone
4,5,7,7a-Tetrahydro-4,4,7a-trimethyl-2(6H)benzofuranone
4,4,7a-Trimethyl-5,6,7,7a-tetrahydro-4H-Benzofuran-2-one
5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone
(2,6,6-trimethy1-2-hydroxycyclohexylidene)-acetic acid lactone
5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-4H-benzo[b]furan-2-one
Dihydroactinolide
5,6,7,7a-tetrahydro-4,4,7a-trimethylbenzofuran-2(4H)-one

Inchi: InChI=1S/C11H16O2/c1-10(2)5-4-6-11(3)8(10)7-9(12)13-11/h7H,4-6H2,1-3H3

InchiKey: IMKHDCBNRDRUEB-UHFFFAOYSA-N

Formula: C11H16O2

SMILES: CC1(C)CCCC2(C)OC(=O)C=C12

Mol. weight [g/mol]: 180.24

CAS: 15356-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-72.42	kJ/mol	Joback Method
hf	-336.16	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	47.83	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.438		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1537.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2332.00		NIST Webbook
tb	576.76	K	Joback Method
tc	823.41	K	Joback Method
tf	394.92	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	576.76	Joback Method
cpg	401.95	J/mol×K	617.87	Joback Method
cpg	418.65	J/mol×K	658.98	Joback Method
cpg	434.48	J/mol×K	700.08	Joback Method
cpg	449.74	J/mol×K	741.19	Joback Method
cpg	464.70	J/mol×K	782.30	Joback Method
cpg	479.66	J/mol×K	823.41	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15356748&Units=SI

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