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

Other names: 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-
Actinidiolide, dihydro-
NSC 357087
Dihydroactinidiolide
4,4,7a-Trimethyl-5,6,7,7a-tetrahydro-1-benzofuran-2(4H)-one, (R)-
5,6,7,7a-Tetrahydro-4,4-7a-trimethyl-2-(4H)-benzofuranone
dihydroactindiolide
5,6,7,7a-Tetrahydro-4,4-7a-trimethyl-2-(4H)-benzofuranone (dihydroactinidiolide)

Inchi: InChI=1S/C11H16O2/c1-10(2)5-4-6-11(3)8(10)7-9(12)13-11/h7H,4-6H2,1-3H3/t11-/m0/s1

InchiKey: IMKHDCBNRDRUEB-NSHDSACASA-N

Formula: $C_{11}H_{16}O_2$

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

Mol. weight [g/mol]: 180.24

CAS: 17092-92-1

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	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1538.00		NIST Webbook

rinpol	1531.00	NIST Webbook
rinpol	1542.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1539.00	NIST Webbook
rinpol	1486.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1490.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1480.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1548.00	NIST Webbook
rinpol	1550.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1485.00	NIST Webbook
rinpol	1537.00	NIST Webbook
rinpol	1539.00	NIST Webbook
rinpol	1539.00	NIST Webbook
rinpol	1532.00	NIST Webbook
rinpol	1538.00	NIST Webbook
rinpol	1499.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1475.00	NIST Webbook
rinpol	1495.00	NIST Webbook
rinpol	1473.00	NIST Webbook
rinpol	1483.00	NIST Webbook
rinpol	1548.00	NIST Webbook
rinpol	1473.00	NIST Webbook
rinpol	1532.00	NIST Webbook
rinpol	1493.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1508.00	NIST Webbook
ripol	2291.00	NIST Webbook
ripol	2291.00	NIST Webbook
ripol	2359.00	NIST Webbook
ripol	2359.00	NIST Webbook
ripol	2280.00	NIST Webbook
ripol	2337.00	NIST Webbook
ripol	2315.00	NIST Webbook
ripol	2354.00	NIST Webbook
ripol	2308.00	NIST Webbook

ripol	2348.00		NIST Webbook
ripol	2324.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2355.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2294.00		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=C17092921&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

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