4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a«alpha»,4«beta»,4a«beta»,7«alpha»,7a«b

Other names: (1aR,4S,4aS,7R,7aS,7bR)-1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulen-4a-ol
4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, (1aR,4S,4aS,7R,7aS,7bR)-
Palustrol
Palustrol (Ledum)
4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-
Diepi-palustrol

Inchi: InChI=1S/C15H26O/c1-9-7-8-15(16)10(2)5-6-11-13(12(9)15)14(11,3)4/h9-13,16H,5-8H2,

InchiKey: QWRTXOOFEHOROQ-UHFFFAOYSA-N

Formula: C15H26O

SMILES: CC1CCC2(O)C(C)CCC3C(C12)C3(C)C

Mol. weight [g/mol]: 222.37

CAS: 5986-49-2

Physical Properties

Property code	Value	Unit	Source
gf	54.83	kJ/mol	Joback Method
hf	-349.96	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1571.00		NIST Webbook

rinpol	1569.00	NIST Webbook
rinpol	1563.00	NIST Webbook
rinpol	1570.00	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1564.00	NIST Webbook
rinpol	1548.00	NIST Webbook
rinpol	1563.00	NIST Webbook
rinpol	1562.00	NIST Webbook
rinpol	1562.00	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1556.00	NIST Webbook
rinpol	1571.00	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1561.00	NIST Webbook
rinpol	1567.00	NIST Webbook
rinpol	1566.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1956.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1931.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1932.00	NIST Webbook
ripol	1956.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1934.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1931.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1928.00	NIST Webbook
ripol	1915.00	NIST Webbook
ripol	1903.00	NIST Webbook
ripol	1931.00	NIST Webbook
ripol	1934.00	NIST Webbook
ripol	1934.00	NIST Webbook
ripol	1934.00	NIST Webbook

ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1885.00		NIST Webbook
tb	645.34	K	Joback Method
tc	851.43	K	Joback Method
tf	397.25	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.58	J/mol×K	645.34	Joback Method
cpg	621.09	J/mol×K	679.69	Joback Method
cpg	640.66	J/mol×K	714.04	Joback Method
cpg	659.50	J/mol×K	748.38	Joback Method
cpg	677.83	J/mol×K	782.73	Joback Method
cpg	695.86	J/mol×K	817.08	Joback Method
cpg	713.82	J/mol×K	851.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5986492&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
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