Cedrol

Other names: (+)-cedrol
(3R,3aS,6R,7R,8aS)-3,6,8,8-tetramethyloctahydro-1H-3a,7-methanoazulen-6-ol
1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-,
[3R-(3«alpha»,3a«beta»,6«alpha»,7«beta»,8a«alpha»)]-
8«beta»H-Cedran-8-ol
[3R-(3«alpha»,3a«beta»,6«alpha»,7«beta»,8a«alpha»)]-octahydro-3,6,8,8-tetramethyl-1H
«alpha»-Cedrol

Inchi: InChI=1S/C15H26O/c1-10-5-6-11-13(2,3)12-9-15(10,11)8-7-14(12,4)16/h10-12,16H,5-9H

InchiKey: SVURIXNDRWRAFU-WINGCZCQSA-N

Formula: C15H26O

SMILES: CC1CCC2C(C)(C)C3CC12CCC3(C)O

Mol. weight [g/mol]: 222.37

CAS: 77-53-2

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1607.90		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1605.80		NIST Webbook

rinpol	1603.00	NIST Webbook
rinpol	1582.00	NIST Webbook
rinpol	1598.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1575.00	NIST Webbook
rinpol	1599.00	NIST Webbook
rinpol	1596.00	NIST Webbook
rinpol	1604.00	NIST Webbook
rinpol	1599.00	NIST Webbook
rinpol	1594.32	NIST Webbook
rinpol	1596.87	NIST Webbook
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rinpol	1612.00	NIST Webbook
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rinpol	1586.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1622.00	NIST Webbook
rinpol	1618.50	NIST Webbook
rinpol	1601.00	NIST Webbook
rinpol	1583.00	NIST Webbook
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rinpol	1616.00	NIST Webbook
rinpol	1574.00	NIST Webbook
rinpol	1596.00	NIST Webbook
rinpol	1609.00	NIST Webbook
rinpol	1600.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1599.00	NIST Webbook
rinpol	1596.87	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1601.00	NIST Webbook
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rinpol	1596.00	NIST Webbook
rinpol	1601.00	NIST Webbook
rinpol	1589.60	NIST Webbook
rinpol	1602.00	NIST Webbook
rinpol	1595.00	NIST Webbook

ripol	2119.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2112.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2112.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2134.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2092.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	359.15	K	Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of vaporization enthalpies and liquid vapor pressures of cedrol, nerolidol, and 1-adamantanol by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2017.07.018
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