Carotol

Other names:	3a(1H)-Azulenol, 2,3,4,5,8,8a-hexahydro-6,8a-dimethyl-3-(1-methylethyl)-, [3R-(3«alpha»,3a«alpha»,8a«alpha»)]- 3a«alpha»(1H)-Azulenol, 2,3,4,5,8,8a-hexahydro-3«alpha»-isopropyl-6,8a«alpha»-dimethyl-, (+)- (+)-Carotol Carotol, (+)- cis-Dauc-8-en-5«beta»-ol cis-Dauc-8-en-5«beta»-ol (Carotol)
Inchi:	InChI=1S/C15H26O/c1-11(2)13-7-9-14(4)8-5-12(3)6-10-15(13,14)16/h5,11,13,16H,6-10H
InchiKey:	XZYQCFABZDVOPN-ILXRZTDVSA-N
Formula:	C15H26O
SMILES:	CC1=CCC2(C)CCC(C(C)C)C2(O)CC1
Mol. weight [g/mol]:	222.37
CAS:	465-28-1

Physical Properties

Property code	Value	Unit	Source
gf	10.90	kJ/mol	Joback Method
hf	-333.03	kJ/mol	Joback Method
hfus	12.35	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1612.30		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1612.30		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1595.00		NIST Webbook

rinpol	1590.00	NIST Webbook
rinpol	1590.00	NIST Webbook
rinpol	1593.00	NIST Webbook
rinpol	1596.00	NIST Webbook
rinpol	1587.00	NIST Webbook
rinpol	1587.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1574.00	NIST Webbook
rinpol	1596.00	NIST Webbook
rinpol	1573.00	NIST Webbook
rinpol	1552.00	NIST Webbook
rinpol	1568.00	NIST Webbook
rinpol	1560.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1600.00	NIST Webbook
rinpol	1600.00	NIST Webbook
rinpol	1568.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1614.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1598.00	NIST Webbook
rinpol	1603.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1590.00	NIST Webbook
rinpol	1573.00	NIST Webbook
rinpol	1600.00	NIST Webbook
rinpol	1591.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	2011.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	2033.00	NIST Webbook
ripol	2024.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2026.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2014.00	NIST Webbook

ripol	2011.00		NIST Webbook
tb	664.85	K	Joback Method
tc	877.11	K	Joback Method
tf	383.27	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.44	J/mol×K	664.85	Joback Method
cpg	611.95	J/mol×K	700.23	Joback Method
cpg	630.65	J/mol×K	735.60	Joback Method
cpg	648.74	J/mol×K	770.98	Joback Method
cpg	666.45	J/mol×K	806.36	Joback Method
cpg	683.99	J/mol×K	841.73	Joback Method
cpg	701.57	J/mol×K	877.11	Joback Method

Sources

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=C465281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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