Daucol

Other names: 1H-3a,6-Epoxyazulen-7-ol, octahydro-6,8a-dimethyl-3-(1-methylethyl)-, [3R-(3«alpha»,3a«alpha»,6«alpha»,7«beta»,8a«alpha»)]-
1H-3a,6-Epoxyazulen-7-ol, 2,3,4,5,6,7«alpha»,8,8a-octahydro-3«alpha»-isopropyl-6«beta»,8a«alpha»-dimethyl-, (-)-
cis-5«beta»,8«beta»-Epoxydaucan-9«alpha»-ol
cis-5«beta»,8«beta»-Epoxydaucan-9«alpha»-ol (Daucol)

Inchi: InChI=1S/C15H26O2/c1-10(2)11-5-6-13(3)9-12(16)14(4)7-8-15(11,13)17-14/h10-12,16H

InchiKey: VLIUMVVQGMLOJG-DRWKLNATSA-N

Formula: C15H26O2

SMILES: CC(C)C1CCC2(C)CC(O)C3(C)CCC12O3

Mol. weight [g/mol]: 238.37

CAS: 887-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-431.32	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.131		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1646.60		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1646.60		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1638.00		NIST Webbook
ripol	2292.00		NIST Webbook
ripol	2284.00		NIST Webbook
ripol	2284.00		NIST Webbook
tb	681.43	K	Joback Method
tc	896.88	K	Joback Method
tf	441.20	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.32	J/mol×K	681.43	Joback Method
cpg	647.61	J/mol×K	717.34	Joback Method
cpg	666.42	J/mol×K	753.25	Joback Method
cpg	685.08	J/mol×K	789.15	Joback Method
cpg	703.94	J/mol×K	825.06	Joback Method
cpg	723.34	J/mol×K	860.97	Joback Method
cpg	743.64	J/mol×K	896.88	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=C887081&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