Taynudol

Other names:	2,8-Dimethyl-5-methylene-2a,3,4,5,5a,6,7,8,8a,8b-decahydro-cyclobuta[e]azulen-4-ol
Inchi:	InChI=1S/C15H22O/c1-8-4-5-11-10(3)14(16)7-12-9(2)6-13(12)15(8)11/h6,8,11-16H,3-5,7
InchiKey:	YHSVQXCYEKUOFR-MQNDFEPXSA-N
Formula:	C15H22O
SMILES:	C=C1C(O)CC2C(C)=CC2C2C(C)CCC12
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	134.83	kJ/mol	Joback Method
hf	-235.71	kJ/mol	Joback Method
hfus	29.69	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.162		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1707.00		NIST Webbook
tb	657.10	K	Joback Method
tc	859.62	K	Joback Method
tf	377.13	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.04	J/mol×K	657.10	Joback Method
cpg	646.18	J/mol×K	825.86	Joback Method
cpg	631.33	J/mol×K	792.11	Joback Method
cpg	615.55	J/mol×K	758.36	Joback Method
cpg	598.78	J/mol×K	724.61	Joback Method
cpg	580.97	J/mol×K	690.85	Joback Method
cpg	660.15	J/mol×K	859.62	Joback Method

dvisc	0.0006461	Pa×s	657.10	Joback Method
dvisc	0.0007686	Pa×s	610.44	Joback Method
dvisc	0.0009410	Pa×s	563.78	Joback Method
dvisc	0.0011949	Pa×s	517.12	Joback Method
dvisc	0.0015909	Pa×s	470.45	Joback Method
dvisc	0.0022560	Pa×s	423.79	Joback Method
dvisc	0.0034881	Pa×s	377.13	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=R407784&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/69-375-0/Taynudol.pdf
Generated by Cheméo on 2024-10-12 02:32:27.845691709 +0000 UTC m=+3281210.482660957.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.