

Cedran-diol, (8S,14)-

Other names:	1H-3a,7-Methanoazulene-8-methanol, octahydro-6-hydroxy-3,6,8-trimethyl-, [3R-(3«alpha»,3a«beta»,6«beta»,7«beta»,8«alpha»,8a«alpha»)]-8S,14-Cedrandiol
Inchi:	InChI=1S/C15H26O2/c1-10-4-5-11-13(2,9-16)12-8-15(10,11)7-6-14(12,3)17/h10-12,16-1
InchiKey:	YULHLOUAHSEHLD-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CC1CCC2C(C)(CO)C3CC12CCC3(C)O
Mol. weight [g/mol]:	238.37
CAS:	62600-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-466.61	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.582		Crippen Method
mvol	201.370	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
tb	742.43	K	Joback Method
tc	943.89	K	Joback Method
tf	486.21	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.89	J/molxK	742.43	Joback Method
cpg	681.70	J/molxK	776.01	Joback Method
cpg	699.55	J/molxK	809.58	Joback Method
cpg	717.73	J/molxK	843.16	Joback Method
cpg	736.52	J/molxK	876.74	Joback Method
cpg	756.20	J/molxK	910.31	Joback Method
cpg	777.05	J/molxK	943.89	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=C62600059&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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