

1H-Inden-4,7-diol, 2,4,5,6,7,7a-hexahydro-2,7-dimethyl-5-methylene-

Inchi: InChI=1S/C15H22O3/c1-9-11(16)15-7-12(2,8-18-15)6-10(15)13(3,17)14(9)4-5-14/h10-11
InchiKey: YOYARHPUJHXQS-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: C=C1C(O)C23CC(C)(CO2)CC3C(C)(O)C12CC2
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-37.74	kJ/mol	Joback Method
hf	-399.83	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	81.61	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.634		Crippen Method
mcvol	192.080	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1788.00		NIST Webbook
ripol	2931.00		NIST Webbook
ripol	2931.00		NIST Webbook
tb	775.92	K	Joback Method
tc	988.95	K	Joback Method
tf	576.06	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.85	J/mol×K	775.92	Joback Method
cpg	660.31	J/mol×K	811.43	Joback Method
cpg	678.83	J/mol×K	846.93	Joback Method
cpg	698.86	J/mol×K	882.44	Joback Method
cpg	720.83	J/mol×K	917.94	Joback Method
cpg	745.20	J/mol×K	953.45	Joback Method
cpg	772.40	J/mol×K	988.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R546453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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