(1S,5R,6S,7R,10R)-Lemnalone

Inchi: InChI=1S/C15H22O/c1-8(2)10-5-6-15(4)11-7-12(16)9(3)14(15)13(10)11/h8,10-11,13-14H
InchiKey: ONOKHKGIKQEZKP-DVHHUASFSA-N
Formula: C15H22O
SMILES: C=C1C(=O)CC2C3C(C(C)C)CCC2(C)C13
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	152.71	kJ/mol	Joback Method
hf	-224.87	kJ/mol	Joback Method
hfus	17.58	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.450		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	624.53	K	Joback Method
tc	850.22	K	Joback Method
tf	391.43	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.86	J/mol×K	624.53	Joback Method
cpg	564.34	J/mol×K	662.14	Joback Method
cpg	584.59	J/mol×K	699.76	Joback Method
cpg	603.78	J/mol×K	737.37	Joback Method
cpg	622.09	J/mol×K	774.99	Joback Method
cpg	639.69	J/mol×K	812.60	Joback Method
cpg	656.73	J/mol×K	850.22	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R561709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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