

Liguloxide

Inchi: InChI=1S/C15H26O/c1-10-5-7-12-9-15(16-14(12,3)4)11(2)6-8-13(10)15/h10-13H,5-9H2,
InchiKey: GXMJXGUEPXEOGR-HLAQNLCESA-N
Formula: C15H26O
SMILES: CC1CCC2CC3(OC2(C)C)C(C)CCC13
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	101.14	kJ/mol	Joback Method
hf	-315.55	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1505.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1532.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1808.00		NIST Webbook
tb	589.05	K	Joback Method
tc	816.69	K	Joback Method
tf	363.72	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/mol×K	589.05	Joback Method
cpg	586.42	J/mol×K	626.99	Joback Method
cpg	609.68	J/mol×K	664.93	Joback Method
cpg	631.66	J/mol×K	702.87	Joback Method
cpg	652.64	J/mol×K	740.81	Joback Method
cpg	672.91	J/mol×K	778.75	Joback Method
cpg	692.75	J/mol×K	816.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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