

Artedouglasia oxide A

Other names:	Artedouglasia oxide A A-Artedouglasia oxide
Inchi:	InChI=1S/C15H22O3/c1-6-14(4)10-8-12(17-14)15(5)11(16)7-9-13(2,3)18-15/h6-7,9,12H,
InchiKey:	YDGSUVJUYWCJCE-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	<chem>C=CC1(C)CCC(C2(C)OC(C)(C)C=CC2=O)O1</chem>
Mol. weight [g/mol]:	250.33
CAS:	115403-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-72.50	kJ/mol	Joback Method
hf	-451.58	kJ/mol	Joback Method
hfus	19.03	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.803		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1542.50		NIST Webbook
rinpol	1541.70		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	686.37	K	Joback Method
tc	938.78	K	Joback Method
tf	460.67	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.71	J/mol×K	686.37	Joback Method
cpg	627.81	J/mol×K	728.44	Joback Method
cpg	649.33	J/mol×K	770.51	Joback Method
cpg	670.71	J/mol×K	812.57	Joback Method
cpg	692.36	J/mol×K	854.64	Joback Method
cpg	714.72	J/mol×K	896.71	Joback Method
cpg	738.19	J/mol×K	938.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115403968&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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