Incensole oxide

Other names: 1-Isopropyl-5,9,13-trimethyl-4,16-dioxatricyclo[11.2.1.03,5]hexadec-8-en-12-ol
Inchi: InChI=1S/C20H34O3/c1-14(2)20-12-11-18(4,23-20)16(21)9-8-15(3)7-6-10-19(5)17(13-20
InchiKey: ARTVDMKLQDTMGX-CHHVJCJISA-N
Formula: C20H34O3
SMILES: CC1=CCCC2(C)OC2CC2(C(C)C)CCC(C)(O2)C(O)C1
Mol. weight [g/mol]: 322.48
CAS: 21698-66-8

Physical Properties

Property code	Value	Unit	Source
gf	-104.31	kJ/mol	Joback Method
hf	-624.21	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	80.85	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.989		Crippen Method
mcvol	259.300	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	2294.20		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	821.12	K	Joback Method
tc	1047.97	K	Joback Method
tf	512.05	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.77	J/mol×K	821.12	Joback Method
cpg	910.38	J/mol×K	858.93	Joback Method
cpg	935.38	J/mol×K	896.74	Joback Method
cpg	961.15	J/mol×K	934.54	Joback Method
cpg	988.05	J/mol×K	972.35	Joback Method
cpg	1016.46	J/mol×K	1010.16	Joback Method

cpg	1046.75	J/mol×K	1047.97	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=C21698668&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