«alpha»-13 oxy-14-en-epilabdane

Inchi: InChI=1S/C20H36O/c1-7-19(5,21)14-11-16-15(2)9-10-17-18(3,4)12-8-13-20(16,17)6/h7,1
InchiKey: FLVAXXPTIPADIG-QBNJSCLLSA-N
Formula: C20H36O
SMILES: C=CC(C)(O)CCC1C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 292.50

Physical Properties

Property code	Value	Unit	Source
gf	110.37	kJ/mol	Joback Method
hf	-401.26	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.582		Crippen Method
mcvol	272.510	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
ripol	2396.00		NIST Webbook
ripol	2396.00		NIST Webbook
tb	759.66	K	Joback Method
tc	965.92	K	Joback Method
tf	433.52	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.93	J/mol×K	759.66	Joback Method
cpg	910.13	J/mol×K	794.04	Joback Method
cpg	932.71	J/mol×K	828.41	Joback Method
cpg	954.90	J/mol×K	862.79	Joback Method
cpg	976.92	J/mol×K	897.17	Joback Method
cpg	999.00	J/mol×K	931.55	Joback Method
cpg	1021.35	J/mol×K	965.92	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=R332586&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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