trans-«alpha»-ambrinol

Inchi: InChI=1S/C13H22O/c1-12(2)7-4-5-10-9-13(3,14)8-6-11(10)12/h5,11,14H,4,6-9H2,1-3H3/
InchiKey: GPVOTKFXWGURGP-YUZLPWPTSA-N
Formula: C13H22O
SMILES: CC1(O)CCC2C(=CCCC2(C)C)C1
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	-3.50	kJ/mol	Joback Method
hf	-286.47	kJ/mol	Joback Method
hfus	10.69	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.284		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1412.00		NIST Webbook
tb	619.53	K	Joback Method
tc	834.63	K	Joback Method
tf	375.73	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.50	J/mol×K	619.53	Joback Method
cpg	503.70	J/mol×K	655.38	Joback Method
cpg	520.97	J/mol×K	691.23	Joback Method
cpg	537.51	J/mol×K	727.08	Joback Method
cpg	553.54	J/mol×K	762.93	Joback Method
cpg	569.27	J/mol×K	798.78	Joback Method
cpg	584.92	J/mol×K	834.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333589&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

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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