Actinidol ethyl ether (isomer I)

Inchi: InChI=1S/C15H24O2/c1-6-16-11(2)12-10-13-14(3,4)8-7-9-15(13,5)17-12/h7,9-12H,6,8H2
InchiKey: VMHZYBPNRMMKGA-QOZQQMKHSA-N
Formula: C15H24O2
SMILES: CCOC(C)C1C=C2C(C)(C)CC=CC2(C)O1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-1.34	kJ/mol	Joback Method
hf	-381.08	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	54.49	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.481		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
ripol	1732.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	616.93	K	Joback Method
tc	835.87	K	Joback Method
tf	375.53	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.43	J/mol×K	616.93	Joback Method
cpg	581.58	J/mol×K	653.42	Joback Method
cpg	600.68	J/mol×K	689.91	Joback Method
cpg	618.95	J/mol×K	726.40	Joback Method
cpg	636.63	J/mol×K	762.89	Joback Method
cpg	653.93	J/mol×K	799.38	Joback Method
cpg	671.07	J/mol×K	835.87	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=R302624&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