[1R-[1«alpha»,3«alpha»,4«beta»]]-4-Ethenyl-«alph

Inchi: InChI=1S/C15H26O/c1-7-15(6)9-8-12(14(4,5)16)10-13(15)11(2)3/h7,12-13,16H,1-2,8-10
InchiKey: GFJIQNADMLPFOW-VNHYZAJKSA-N
Formula: C15H26O
SMILES: C=CC1(C)CCC(C(C)(C)O)CC1C(=C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	112.11	kJ/mol	Joback Method
hf	-243.96	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1556.30		NIST Webbook
rinpol	1553.40		NIST Webbook
rinpol	1552.40		NIST Webbook
tb	635.24	K	Joback Method
tc	836.45	K	Joback Method
tf	327.37	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.75	J/mol×K	635.24	Joback Method
cpg	607.17	J/mol×K	668.78	Joback Method
cpg	625.55	J/mol×K	702.31	Joback Method
cpg	642.99	J/mol×K	735.85	Joback Method
cpg	659.62	J/mol×K	769.38	Joback Method
cpg	675.56	J/mol×K	802.92	Joback Method
cpg	690.93	J/mol×K	836.45	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=R419400&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