trans-Arteannuic alcohol

Inchi: InChI=1S/C15H24O/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)15(13)8-10/h8,11,13-16H,3-7,9
InchiKey: CZSSHKCZSDDOAH-CMAYJEJSSA-N
Formula: C15H24O
SMILES: C=C(CO)C1CCC(C)C2CCC(C)=CC12
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	95.90	kJ/mol	Joback Method
hf	-262.93	kJ/mol	Joback Method
hfus	26.95	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.554		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	656.70	K	Joback Method
tc	858.12	K	Joback Method
tf	330.51	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.43	J/mol×K	656.70	Joback Method
cpg	596.86	J/mol×K	690.27	Joback Method
cpg	615.17	J/mol×K	723.84	Joback Method
cpg	632.38	J/mol×K	757.41	Joback Method
cpg	648.56	J/mol×K	790.98	Joback Method
cpg	663.74	J/mol×K	824.55	Joback Method

cpg	677.97	J/mol×K	858.12	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=R625328&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