trans-Arteannuic alcohol

Inchi: InChI=1S/C15H26O/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)15(13)8-10/h8,11-16H,4-7,9H2,
InchiKey: SIKURLYPEUHJFQ-NUZWPGIQSA-N
Formula: C15H26O
SMILES: CC1=CC2C(C(C)CO)CCC(C)C2CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	14.17	kJ/mol	Joback Method
hf	-383.85	kJ/mol	Joback Method
hfus	26.02	kJ/mol	Joback Method
hvap	66.12	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.633		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1582.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1999.00		NIST Webbook
tb	659.70	K	Joback Method
tc	858.28	K	Joback Method
tf	331.23	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.30	J/mol×K	659.70	Joback Method
cpg	621.31	J/mol×K	692.80	Joback Method
cpg	640.20	J/mol×K	725.89	Joback Method
cpg	657.98	J/mol×K	758.99	Joback Method

cpg	674.70	J/mol×K	792.09	Joback Method
cpg	690.40	J/mol×K	825.19	Joback Method
cpg	705.12	J/mol×K	858.28	Joback Method
dvisc	0.0069291	Pa×s	331.23	Joback Method
dvisc	0.0022185	Pa×s	385.98	Joback Method
dvisc	0.0009426	Pa×s	440.72	Joback Method
dvisc	0.0004839	Pa×s	495.47	Joback Method
dvisc	0.0002837	Pa×s	550.21	Joback Method
dvisc	0.0001831	Pa×s	604.96	Joback Method
dvisc	0.0001272	Pa×s	659.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200152&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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