Davanol (isomer)

Inchi: InChI=1S/C15H26O2/c1-6-15(5)10-9-14(17-15)12(4)13(16)8-7-11(2)3/h6-7,12-14,16H,1,
InchiKey: XDDCIEBLDYBJNU-NEXFUWMNSA-N
Formula: C15H26O2
SMILES: C=CC1(C)CCC(C(C)C(O)CC=C(C)C)O1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	30.46	kJ/mol	Joback Method
hf	-359.48	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.463		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1591.00		NIST Webbook
tb	672.42	K	Joback Method
tc	868.02	K	Joback Method
tf	325.96	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.62	J/mol×K	672.42	Joback Method
cpg	635.10	J/mol×K	705.02	Joback Method
cpg	651.78	J/mol×K	737.62	Joback Method
cpg	667.76	J/mol×K	770.22	Joback Method
cpg	683.16	J/mol×K	802.82	Joback Method
cpg	698.09	J/mol×K	835.42	Joback Method
cpg	712.67	J/mol×K	868.02	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=R89552&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