amorph-4-en-10«beta»-ol

Inchi: InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-
InchiKey: LHYHMMRYTDARSZ-PPWQZUPISA-N
Formula: C15H26O
SMILES: CC1=CC2C(C(C)C)CCC(C)(O)C2CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hf	-285.47	kJ/mol	Cheméo Relay (1.0)
hfus	19.72	kJ/mol	Joback Method
hvap	82.40	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
tb	557.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method
cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R500739&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature