8«alpha»,11-Elemodiol

Inchi: InChI=1S/C14H24O2/c1-6-10-7-13(15)12(14(4,5)16)8-11(10)9(2)3/h6,10-13,15-16H,1-2,
InchiKey: QKVCTWTVHSDDGI-HNGCFSAESA-N
Formula: C14H24O2
SMILES: C=CC1CC(O)C(C(C)(C)O)CC1C(=C)C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
hfus	23.96	kJ/mol	Joback Method
logp	2.523		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.92	J/mol×K	699.63	Joback Method
cpg	624.07	J/mol×K	730.97	Joback Method
cpg	639.28	J/mol×K	762.32	Joback Method
cpg	653.59	J/mol×K	793.66	Joback Method
cpg	667.04	J/mol×K	825.01	Joback Method
cpg	679.68	J/mol×K	856.35	Joback Method
cpg	691.53	J/mol×K	887.69	Joback Method

Sources

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=R633359&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices