«beta»-epi-Acorenol

Inchi: InChI=1S/C15H26O/c1-11-7-9-15(10-8-11)12(2)5-6-13(15)14(3,4)16/h7,12-13,16H,5-6,8-
InchiKey: XDVDHFJMCJWDPI-RMTCENKZSA-N
Formula: C15H26O
SMILES: CC1=CCC2(CC1)C(C)CCC2C(C)(C)O
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	14.76	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2105.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.13	J/mol×K	661.82	Joback Method
cpg	618.08	J/mol×K	697.19	Joback Method
cpg	636.92	J/mol×K	732.57	Joback Method
cpg	654.81	J/mol×K	767.94	Joback Method
cpg	671.91	J/mol×K	803.32	Joback Method
cpg	688.38	J/mol×K	838.69	Joback Method
cpg	704.35	J/mol×K	874.07	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613479&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

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
ripol:	Polar retention indices