«alpha»-Bisabolene epoxide

Inchi: InChI=1S/C15H24O/c1-11(2)5-10-14-15(4,16-14)13-8-6-12(3)7-9-13/h5-6,13-14H,7-10H2
InchiKey: PBNXUEQZNAEDOI-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=CCC1OC1(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	27.05	kJ/mol	Joback Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1531.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.36	J/mol×K	599.59	Joback Method
cpg	556.81	J/mol×K	636.23	Joback Method
cpg	576.95	J/mol×K	672.87	Joback Method
cpg	595.97	J/mol×K	709.51	Joback Method
cpg	614.03	J/mol×K	746.15	Joback Method
cpg	631.29	J/mol×K	782.79	Joback Method
cpg	647.92	J/mol×K	819.43	Joback Method

Sources

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
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R609960&Units=SI

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