trans-Z-«alpha»-Bisabolene epoxide

Inchi: InChI=1S/C15H24O/c1-11(2)6-5-7-12(3)13-8-9-15(4)14(10-13)16-15/h6-7,13-14H,5,8-10
InchiKey: BOWJPMUUGHPAAF-GHXNOFRVSA-N
Formula: C15H24O
SMILES: CC(C)=CCC=C(C)C1CCC2(C)OC2C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	29.31	kJ/mol	Joback Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.18	J/mol×K	590.95	Joback Method
cpg	552.95	J/mol×K	626.84	Joback Method
cpg	572.39	J/mol×K	662.73	Joback Method
cpg	590.70	J/mol×K	698.61	Joback Method
cpg	608.08	J/mol×K	734.50	Joback Method
cpg	624.71	J/mol×K	770.39	Joback Method
cpg	640.78	J/mol×K	806.28	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131711&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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