

trans-(Z)-«alpha»-Bisabolene oxide

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,7-10H
InchiKey:	PBNXUEQZNAEDOI-JVIGXAJISA-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	1533.00		NIST Webbook
rinpol	1533.00		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

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=R639817&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>

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

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