

«alpha»-Bisabolene oxide

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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,15H

PBNXUEQZNAEDOI-UHFFFAOYSA-N

C15H24O

CC(C)=CCC1OC1(C)C1CC=C(C)CC1

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	1672.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1670.00		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

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=R231864&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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