ISOLONGIFOLENE OXIDE

Other names: octahydro-4,4,8,8-tetramethyl-4a,7-methano-4aH-naphth[1,8a-b]oxirene
Inchi: InChI=1S/C15H24O/c1-12(2)7-6-11-15(16-11)13(3,4)10-5-8-14(12,15)9-10/h10-11H,5-9H
InchiKey: VQHLGZRKOZIABH-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1(C)CCC2OC23C(C)(C)C2CCC13C2
Mol. weight [g/mol]: 220.36

Physical Properties

Property code	Value	Unit	Source
hfus	12.07	kJ/mol	Joback Method
logp	3.770		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
rinpol	1544.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.28	J/mol×K	588.13	Joback Method
cpg	560.07	J/mol×K	627.95	Joback Method
cpg	580.30	J/mol×K	667.77	Joback Method
cpg	599.60	J/mol×K	707.59	Joback Method
cpg	618.63	J/mol×K	747.41	Joback Method
cpg	638.01	J/mol×K	787.23	Joback Method
cpg	658.40	J/mol×K	827.05	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=C67999568&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