

trans-«beta»-Caryophyllene oxide

Inchi: InChI=1S/C15H24O/c1-10-5-6-13-15(4,16-13)8-7-12-11(10)9-14(12,2)3/h11-13H,1,5-9H2
InchiKey: NVEQFIOZRFFVFW-XPCVCDNBSA-N
Formula: C15H24O
SMILES: C=C1CCC2OC2(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	19.08	kJ/mol	Joback Method
hvap	67.91	kJ/mol	Cheméo Relay (1.0)
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
ripol	1581.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1966.00		NIST Webbook
tb	553.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.37	J/mol×K	592.88	Joback Method
cpg	562.46	J/mol×K	631.15	Joback Method
cpg	584.07	J/mol×K	669.42	Joback Method
cpg	604.52	J/mol×K	707.69	Joback Method
cpg	624.09	J/mol×K	745.96	Joback Method
cpg	643.08	J/mol×K	784.23	Joback Method
cpg	661.78	J/mol×K	822.50	Joback Method

Sources

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=R610247&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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