caryophillan-2,6-«beta»-oxide

Inchi: InChI=1S/C15H26O/c1-13(2)10-12-11(13)6-9-14(3)7-5-8-15(12,4)16-14/h11-12H,5-10H2
InchiKey: FMRYSKILCWLXDC-QEOVQVNQSA-N
Formula: C15H26O
SMILES: CC12CCCC(C)(O1)C1CC(C)(C)C1CC2
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	103.36	kJ/mol	Joback Method
hf	-279.97	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.160		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
ripol	2037.00		NIST Webbook
tb	593.96	K	Joback Method
tc	830.88	K	Joback Method
tf	391.86	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.99	J/mol×K	593.96	Joback Method
cpg	583.21	J/mol×K	633.45	Joback Method
cpg	605.88	J/mol×K	672.93	Joback Method
cpg	627.44	J/mol×K	712.42	Joback Method
cpg	648.34	J/mol×K	751.91	Joback Method
cpg	669.02	J/mol×K	791.40	Joback Method
cpg	689.92	J/mol×K	830.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/72-010-0/caryophillan-2-6-beta-oxide.pdf

Generated by Cheméo on 2024-10-12 03:29:56.38673117 +0000 UTC m=+3284659.023700418.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.