Germacrene D-1,10-epoxide

Inchi: InChI=1S/C16H28O/c1-12(2)15-9-6-13(3)7-11-16(17-5)14(4)8-10-15/h6,9,12,14-16H,3,7-
InchiKey: KCOVYKLMLVCCRK-IMUFZNECSA-N
Formula: C16H28O
SMILES: C=C1C=CC(C(C)C)CCC(C)C(OC)CC1
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	20.07	kJ/mol	Joback Method
hf	-380.05	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	54.18	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.596		Crippen Method
mcvol	222.710	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1700.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2042.00		NIST Webbook
tb	613.07	K	Joback Method
tc	826.72	K	Joback Method
tf	276.57	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.85	J/mol×K	613.07	Joback Method
cpg	632.33	J/mol×K	648.68	Joback Method
cpg	656.41	J/mol×K	684.29	Joback Method

cpg	679.08	J/mol×K	719.90	Joback Method
cpg	700.33	J/mol×K	755.51	Joback Method
cpg	720.12	J/mol×K	791.11	Joback Method
cpg	738.45	J/mol×K	826.72	Joback Method
dvisc	0.0050581	Pa×s	276.57	Joback Method
dvisc	0.0013141	Pa×s	332.65	Joback Method
dvisc	0.0005037	Pa×s	388.74	Joback Method
dvisc	0.0002459	Pa×s	444.82	Joback Method
dvisc	0.0001409	Pa×s	500.90	Joback Method
dvisc	0.0000904	Pa×s	556.99	Joback Method
dvisc	0.0000628	Pa×s	613.07	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R234432&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume