endo-5-Methoxy-«beta»-patchoulene

Inchi: InChI=1S/C16H26O/c1-10-8-13(17-5)14-12(10)9-11-6-7-16(14,4)15(11,2)3/h10-11,13H,6
InchiKey: QZULVJXPAUVVFC-MSIPSHCFSA-N
Formula: C16H26O
SMILES: COC1CC(C)C2=C1C1(C)CCC(C2)C1(C)C
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	121.19	kJ/mol	Joback Method
hf	-275.07	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	52.40	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.184		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	616.92	K	Joback Method
tc	836.49	K	Joback Method
tf	404.21	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.89	J/mol×K	616.92	Joback Method
cpg	609.04	J/mol×K	653.52	Joback Method
cpg	630.03	J/mol×K	690.11	Joback Method
cpg	650.12	J/mol×K	726.71	Joback Method
cpg	669.55	J/mol×K	763.30	Joback Method
cpg	688.59	J/mol×K	799.90	Joback Method

cpg	707.47	J/mol×K	836.49	Joback Method

Sources

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=R642383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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