Unknown Black Pepper Gremacrene-D-4-ol isomer RI 1627

Inchi: InChI=1S/C15H26O/c1-12(2)14-8-7-13(3)6-5-10-15(4,16)11-9-14/h6,9,11-12,14,16H,5,7-

InchiKey: RHCTXHCNRLCYBN-BMCYRRRCSA-N

Formula: C15H26O

SMILES: CC1=CCCC(C)(O)C=CC(C(C)C)CC1

Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-50.70	kJ/mol	Joback Method
hf	-381.77	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1626.90		NIST Webbook
tb	669.84	K	Joback Method
tc	882.46	K	Joback Method
tf	331.63	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.33	J/mol×K	669.84	Joback Method
cpg	615.86	J/mol×K	705.28	Joback Method
cpg	635.31	J/mol×K	740.71	Joback Method
cpg	653.77	J/mol×K	776.15	Joback Method
cpg	671.33	J/mol×K	811.58	Joback Method
cpg	688.06	J/mol×K	847.02	Joback Method
cpg	704.06	J/mol×K	882.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413973&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume