Bergamotol

Inchi: InChI=1S/C15H24O/c1-11(10-16)5-4-8-15(3)13-7-6-12(2)14(15)9-13/h5-6,13-14,16H,4,7
InchiKey: JGINTSAQGRHGMG-KAIHXKKWSA-N
Formula: C15H24O
SMILES: CC(=CCCC1(C)C2CC=C(C)C1C2)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	126.80	kJ/mol	Joback Method
hf	-217.08	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	656.28	K	Joback Method
tc	851.05	K	Joback Method
tf	365.89	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.15	J/mol×K	656.28	Joback Method
cpg	582.77	J/mol×K	688.74	Joback Method
cpg	598.62	J/mol×K	721.20	Joback Method
cpg	613.83	J/mol×K	753.67	Joback Method
cpg	628.52	J/mol×K	786.13	Joback Method
cpg	642.83	J/mol×K	818.59	Joback Method

cpg	656.88	J/mol×K	851.05	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=R229900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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