Bergamotol, Z-«alpha»-trans-

Other names:	5-(2,6-Dimethylbicyclo[3.1.1]hept-2-en-6-yl)-2-methyl-2-penten-1-ol-, [1S-[1a,5a,6a(Z)]]-
	«alpha»-trans-Bergamotenol
	(Z)-«alpha»-trans-Bergamotol
	(Z,E)- «alpha»-Bergamotol
	(Z)-trans- «alpha»-Bergamotol
	trans-(Z)-«alpha»-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-WZUFQYTHSA-N
Formula:	C15H24O
SMILES:	CC(=CCCC1(C)C2CC=C(C)C1C2)CO
Mol. weight [g/mol]:	220.35
CAS:	88034-74-6

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	1697.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1703.00		NIST Webbook
ripol	2328.00		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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88034746&Units=SI

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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