

trans-«beta»-Bergamotene

Inchi:	InChI=1S/C15H24/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6,13-14H,3,5,7-10H2,1
InchiKey:	DGZBGCMPRYFWFF-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=C1CCC2CC1C2(C)CCC=C(C)C</chem>
Mol. weight [g/mol]:	204.35
CAS:	15438-94-5

Physical Properties

Property code	Value	Unit	Source
gf	296.37	kJ/mol	Joback Method
hf	-26.92	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1493.20		NIST Webbook
rinpol	1490.60		NIST Webbook
tb	559.12	K	Joback Method
tc	765.28	K	Joback Method
tf	305.47	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.48	J/molxK	559.12	Joback Method
cpg	516.19	J/molxK	593.48	Joback Method
cpg	535.61	J/molxK	627.84	Joback Method
cpg	553.91	J/molxK	662.20	Joback Method

cpg	571.23	J/mol×K	696.56	Joback Method
cpg	587.73	J/mol×K	730.92	Joback Method
cpg	603.56	J/mol×K	765.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C15438945&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
mvol:	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

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