«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-GRKKQISMSA-N
Formula: C15H24
SMILES: C=C1CCC2CC1C2(C)CCC=C(C)C
Mol. weight [g/mol]: 204.35

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	1425.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1600.00		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/mol×K	559.12	Joback Method
cpg	516.19	J/mol×K	593.48	Joback Method
cpg	535.61	J/mol×K	627.84	Joback Method

cpg	553.91	J/mol×K	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/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=R127527&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