«alpha»-cis-Bergamotene

Inchi: InChI=1S/C15H24/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6-7,13-14H,5,8-10H2,1-
InchiKey: YMBFCQPIMVLNIU-RBSFLKMASA-N
Formula: C15H24
SMILES: CC(C)=CCCC1(C)C2CC=C(C)C1C2
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	23.27	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Cheméo Relay (1.0)
ie	7.90	eV	Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1414.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	536.39	K	Cheméo Relay (1.0)
tf	239.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.98	J/mol×K	564.10	Joback Method
cpg	517.47	J/mol×K	598.66	Joback Method
cpg	536.69	J/mol×K	633.23	Joback Method
cpg	554.80	J/mol×K	667.79	Joback Method
cpg	571.95	J/mol×K	702.35	Joback Method
cpg	588.31	J/mol×K	736.92	Joback Method
cpg	604.03	J/mol×K	771.48	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613568&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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