«alpha»-trans-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-GRKKQISMSA-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	1439.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1437.00		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=R612847&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