

(Z)-«alpha»-trans-Bergamotene

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-KAIHXXKWSA-N
Formula:	C15H24O
SMILES:	CC(=CCCC1(C)C2CC=C(C)C1C2)CO
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	27.36	kJ/mol	Joback Method
hvap	94.11	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
ripol	1573.00		NIST Webbook
ripol	1573.00		NIST Webbook
tb	577.53	K	Cheméo Relay (1.0)
tf	306.29	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R616354&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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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