

«alpha»-trans-«beta»-Bergamotene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

YMBFCQPIMVLNIU-KFWWJZLASA-N

C15H24

CC(C)=CCCC1(C)C2CC=C(C)C1C2

204.35

Physical Properties

Property code	Value	Unit	Source
gf	263.62	kJ/mol	Joback Method
hf	-64.85	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	48.51	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1496.00		NIST Webbook
tb	564.10	K	Joback Method
tc	771.48	K	Joback Method
tf	305.07	K	Joback Method
vc	0.746	m3/kmol	Joback Method

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
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=R313921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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