(E)-trans-«alpha»-bergamota-2,10-dien-12-al

Inchi: InChI=1S/C15H22O/c1-11(10-16)5-4-8-15(3)13-7-6-12(2)14(15)9-13/h5-6,10,13-14H,4,7
InchiKey: QWQJWQIDOZWIKY-AKZWGNFOSA-N
Formula: C15H22O
SMILES: CC(C=O)=CCCC1(C)C2CC=C(C)C1C2
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	164.10	kJ/mol	Joback Method
hf	-150.43	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1675.00		NIST Webbook
tb	612.76	K	Joback Method
tc	822.99	K	Joback Method
tf	347.07	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.36	J/mol×K	612.76	Joback Method
cpg	541.68	J/mol×K	647.80	Joback Method
cpg	558.94	J/mol×K	682.84	Joback Method
cpg	575.30	J/mol×K	717.88	Joback Method
cpg	590.91	J/mol×K	752.91	Joback Method
cpg	605.95	J/mol×K	787.95	Joback Method
cpg	620.58	J/mol×K	822.99	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=R233617&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume