Aromadendr-1(10)-en-9-one (squamulosone)

Other names: aromadendr-1(10)-en-9-one
Inchi: InChI=1S/C15H22O/c1-8-5-6-10-9(2)12(16)7-11-14(13(8)10)15(11,3)4/h8,11,13-14H,5-7
InchiKey: FUIPJCVSKAWFTI-HRFWHUSOSA-N
Formula: C15H22O
SMILES: CC1=C2CCC(C)C2C2C(CC1=O)C2(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	100.67	kJ/mol	Joback Method
hf	-275.15	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1764.00		NIST Webbook
ripol	2391.00		NIST Webbook
tb	639.20	K	Joback Method
tc	869.72	K	Joback Method
tf	415.03	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/mol×K	639.20	Joback Method
cpg	567.48	J/mol×K	677.62	Joback Method
cpg	587.88	J/mol×K	716.04	Joback Method
cpg	607.27	J/mol×K	754.46	Joback Method
cpg	625.82	J/mol×K	792.88	Joback Method

cpg	643.70	J/mol×K	831.30	Joback Method
cpg	661.06	J/mol×K	869.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228932&Units=SI
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

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

Latest version available from:

https://www.chemeo.com/cid/65-454-6/Aromadendr-1-10-en-9-one-squamulosone.pdf

Generated by Cheméo on 2024-10-12 06:59:56.301567571 +0000 UTC m=+3297258.938536831.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.