Aromandendrene

Other names: 1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a«alpha»,4a«alpha»,7«alpha»,7a«beta»,7b«alpha»)]-
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, (1aR,4aR,7R,7aR,7bS)-(+)-
(1aR,4aR,7R,7aR,7bS)-1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulene
Aromadendr-7(15)-ene
(+)-Aromadendrene
Aromadendrene, (+)-
1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulene-, [1aR-(1a«alpha»,4a«alpha»,7«alpha»,7a«beta»,7b«alpha»)]-
[1aR-(1a«alpha»,4a«alpha»,7«alpha»,7a«beta»,7b«alpha»)]-decahydro-1,1,7-trimethyl-4

Inchi: InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h10-14H,1,5-8H2,2-4H

InchiKey: ITYNGVSTWVVPIC-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C1CCC2C(C3C(C)CCC13)C2(C)C

Mol. weight [g/mol]: 204.35

CAS: 489-39-4

Physical Properties

Property code	Value	Unit	Source
gf	257.93	kJ/mol	Joback Method
hf	-108.39	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1447.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1622.00		NIST Webbook

ripol	1637.00		NIST Webbook
tb	535.50 ± 2.50	K	NIST Webbook
tc	772.11	K	Joback Method
tf	330.45	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.38	J/mol×K	556.75	Joback Method
cpg	527.20	J/mol×K	592.64	Joback Method
cpg	549.51	J/mol×K	628.54	Joback Method
cpg	570.48	J/mol×K	664.43	Joback Method
cpg	590.26	J/mol×K	700.32	Joback Method
cpg	609.03	J/mol×K	736.21	Joback Method
cpg	626.94	J/mol×K	772.11	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=C489394&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume