

Alloaromadendrene

Other names:	1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a«alpha»,4a«beta»,7«alpha»,7a«beta»,7b«alpha»)]- 1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, (1aR,4aS,7R,7aR,7bS)-(-)- (-)-Alloaromadendrene L-Alloaromadendrene Alloaromadendren 1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulene-, [1aR-(1a«alpha»,4a«beta»,7«alpha»,7a«beta»,7b«alpha»)]- Aromadendrene, allo- (1aR,4aS,7R,7aR,7bS)-1,1,7-Trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulene allo-aromandendrene Alloaromadedrene
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:	ITYNGVSTWVVIC-OOAQSJESSA-N
Formula:	C15H24
SMILES:	C=C1CCC2C(C3C(C)CCC13)C2(C)C
Mol. weight [g/mol]:	204.35
CAS:	25246-27-9

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
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ripol	1645.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1636.00		NIST Webbook
tb	556.75	K	Joback Method
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=C25246279&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

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