Dehydroaromadendrene

Other names:	Dehydroaromadendrane
	Aromadendr-9-ene
	9,10-Aromadendrene
	(1a«alpha»,4a«alpha»,7«alpha»,7a«beta»,7b«alpha»)-(-)-1a,2,4a,5,6,7,7a,7b-octahydro-
Inchi:	InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h6,10-14H,5,7-8H2,1-4
InchiKey:	DJAYTQZJAJXFDU-DGOFFYKESA-N
Formula:	C15H24
SMILES:	CC1=CCC2C(C3C(C)CCC13)C2(C)C
Mol. weight [g/mol]:	204.35
CAS:	85048-01-7

Physical Properties

Property code	Value	Unit	Source
gf	225.18	kJ/mol	Joback Method
hf	-146.32	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1462.00		NIST Webbook

rinpol	1442.00		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	561.73	K	Joback Method
tc	778.35	K	Joback Method
tf	330.05	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.21	J/mol×K	561.73	Joback Method
cpg	528.79	J/mol×K	597.83	Joback Method
cpg	550.88	J/mol×K	633.94	Joback Method
cpg	571.64	J/mol×K	670.04	Joback Method
cpg	591.24	J/mol×K	706.14	Joback Method
cpg	609.85	J/mol×K	742.24	Joback Method
cpg	627.64	J/mol×K	778.35	Joback Method

Sources

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=C85048017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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