(-)-Dehydroaromadendrene

Inchi: InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h6,8,10-14H,1,5,7H2,2
InchiKey: OXBYVYGWWRTWMD-UHFFFAOYSA-N
Formula: C15H22
SMILES: C=C1C=CC2C(C3C(C)CCC13)C2(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	287.89	kJ/mol	Joback Method
hf	-50.61	kJ/mol	Joback Method
hfus	21.79	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.047		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	555.91	K	Joback Method
tc	773.35	K	Joback Method
tf	331.21	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.11	J/mol×K	555.91	Joback Method
cpg	506.84	J/mol×K	592.15	Joback Method
cpg	528.08	J/mol×K	628.39	Joback Method
cpg	548.00	J/mol×K	664.63	Joback Method
cpg	566.78	J/mol×K	700.87	Joback Method
cpg	584.58	J/mol×K	737.11	Joback Method
cpg	601.57	J/mol×K	773.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182866&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume