allo-9-aromadendrene

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-DGOFFYKESA-N
Formula: C15H24
SMILES: C=C1CCC2C(C3C(C)CCC13)C2(C)C
Mol. weight [g/mol]: 204.35

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	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238241&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