«beta»-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-DYECWSKSSA-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	1459.00		NIST Webbook
rinpol	1459.00		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=R340968&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume