Isoaromadendrene

Inchi: InChI=1S/C14H22/c1-9-7-8-10-5-4-6-11-13(12(9)10)14(11,2)3/h4-5,9-13H,6-8H2,1-3H3
InchiKey: IHQUEBHATOOKPN-UHFFFAOYSA-N
Formula: C14H22
SMILES: CC1CCC2C=CCC3C(C12)C3(C)C
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	226.39	kJ/mol	Joback Method
hf	-114.21	kJ/mol	Joback Method
hfus	20.36	kJ/mol	Joback Method
hvap	45.05	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.881		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1437.00		NIST Webbook
tb	533.87	K	Joback Method
tc	753.17	K	Joback Method
tf	306.26	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.90	J/mol×K	533.87	Joback Method
cpg	475.68	J/mol×K	570.42	Joback Method
cpg	497.82	J/mol×K	606.97	Joback Method
cpg	518.50	J/mol×K	643.52	Joback Method
cpg	537.89	J/mol×K	680.07	Joback Method
cpg	556.19	J/mol×K	716.62	Joback Method
cpg	573.56	J/mol×K	753.17	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=R574062&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