Isoaromadendrene epoxide

Inchi: InChI=1S/C15H24O/c1-8-5-6-9-12(8)13-10(14(13,2)3)7-11-15(9,4)16-11/h8-13H,5-7H2,1
InchiKey: GLKQAHXBJLGAFT-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1CCC2C1C1C(CC3OC32C)C1(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	190.48	kJ/mol	Joback Method
hf	-244.61	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	49.61	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.482		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1807.00		NIST Webbook
tb	578.31	K	Joback Method
tc	798.81	K	Joback Method
tf	387.98	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.31	J/mol×K	578.31	Joback Method
cpg	566.49	J/mol×K	615.06	Joback Method
cpg	588.09	J/mol×K	651.81	Joback Method
cpg	608.41	J/mol×K	688.56	Joback Method
cpg	627.78	J/mol×K	725.31	Joback Method
cpg	646.49	J/mol×K	762.06	Joback Method
cpg	664.85	J/mol×K	798.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U159366&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