Aromadendrene oxide-(2)

Inchi: InChI=1S/C15H24O/c1-9-4-5-10-12(9)13-11(14(13,2)3)6-7-15(10)8-16-15/h9-13H,4-8H2
InchiKey: XPGWKKLDFXNBPJ-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1CCC2C1C1C(CCC23CO3)C1(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	186.09	kJ/mol	Joback Method
hf	-230.43	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.484		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1678.00		NIST Webbook
ripol	2299.00		NIST Webbook
tb	587.25	K	Joback Method
tc	815.53	K	Joback Method
tf	388.70	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.52	J/mol×K	587.25	Joback Method
cpg	568.21	J/mol×K	625.30	Joback Method
cpg	590.27	J/mol×K	663.34	Joback Method
cpg	611.03	J/mol×K	701.39	Joback Method
cpg	630.84	J/mol×K	739.44	Joback Method
cpg	650.04	J/mol×K	777.48	Joback Method
cpg	668.97	J/mol×K	815.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151986&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

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