«alpha»-Corocalene epoxide

Inchi: InChI=1S/C15H20O/c1-9(2)11-6-5-10(3)12-7-8-15(4)14(16-15)13(11)12/h5-6,9,14H,7-8H
InchiKey: DFKNZQFKCBZNBE-UHFFFAOYSA-N
Formula: C15H20O
SMILES: Cc1ccc(C(C)C)c2c1CCC1(C)OC21
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	198.49	kJ/mol	Joback Method
hf	-121.09	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.895		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
ripol	2337.00		NIST Webbook
ripol	2337.00		NIST Webbook
tb	620.18	K	Joback Method
tc	846.36	K	Joback Method
tf	397.66	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.26	J/mol×K	620.18	Joback Method
cpg	513.05	J/mol×K	657.88	Joback Method
cpg	529.77	J/mol×K	695.57	Joback Method
cpg	545.61	J/mol×K	733.27	Joback Method
cpg	560.80	J/mol×K	770.96	Joback Method
cpg	575.53	J/mol×K	808.66	Joback Method

cpg	590.00	J/mol×K	846.36	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=R229460&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume