Italicene epoxide

Other names: (1aR,1bS,2aS,5S,5aS,7aS)-2,2,5,7a-Tetramethyldecahydrocyclopenta[2',3']cyclobuta[1',2
Inchi: InChI=1S/C15H24O/c1-9-5-6-10-13(2,3)11-12-14(4,16-12)7-8-15(9,10)11/h9-12H,5-8H2,
InchiKey: MSWITNNAHMCECB-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1CCC2C(C)(C)C3C4OC4(C)CCC123
Mol. weight [g/mol]: 220.35
CAS: 104188-24-1

Physical Properties

Property code	Value	Unit	Source
gf	192.70	kJ/mol	Joback Method
hf	-209.03	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.626		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	583.22	K	Joback Method
tc	812.69	K	Joback Method
tf	416.12	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.98	J/mol×K	583.22	Joback Method
cpg	563.50	J/mol×K	621.46	Joback Method
cpg	584.43	J/mol×K	659.71	Joback Method

cpg	604.21	J/mol×K	697.95	Joback Method
cpg	623.32	J/mol×K	736.20	Joback Method
cpg	642.20	J/mol×K	774.44	Joback Method
cpg	661.33	J/mol×K	812.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104188241&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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