Salsolene epoxide

Inchi: InChI=1S/C15H24O/c1-10(2)13-6-7-15-9-12(13)8-11(3)4-5-14(15)16-15/h8,10,12-14H,4-
InchiKey: ZBBZNJBCTBFTGY-FJSNLOIRSA-N
Formula: C15H24O
SMILES: CC1=CC2CC3(CCC2C(C)C)OC3CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	139.94	kJ/mol	Joback Method
hf	-249.08	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1716.00		NIST Webbook
tb	601.85	K	Joback Method
tc	828.55	K	Joback Method
tf	346.58	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.13	J/mol×K	601.85	Joback Method
cpg	565.04	J/mol×K	639.63	Joback Method
cpg	586.46	J/mol×K	677.42	Joback Method
cpg	606.60	J/mol×K	715.20	Joback Method
cpg	625.65	J/mol×K	752.99	Joback Method
cpg	643.82	J/mol×K	790.77	Joback Method
cpg	661.30	J/mol×K	828.55	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=R232812&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