

7-epi-10,11-epoxy-ar-curcumen-15-al

Inchi:	InChI=1S/C15H20O2/c1-11(4-9-14-15(2,3)17-14)13-7-5-12(10-16)6-8-13/h5-8,10-11,14H
InchiKey:	NLFRNGVJOBVJLR-YNODCEANSA-N
Formula:	C15H20O2
SMILES:	CC(CCC1OC1(C)C)c1ccc(C=O)cc1
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
gf	37.67	kJ/mol	Joback Method
hf	-283.03	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.560		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinsol	1815.00		NIST Webbook
tb	651.74	K	Joback Method
tc	870.21	K	Joback Method
tf	388.92	K	Joback Method
vc	0.753	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.57	J/mol×K	651.74	Joback Method
cpg	552.61	J/mol×K	688.15	Joback Method
cpg	568.72	J/mol×K	724.56	Joback Method
cpg	584.06	J/mol×K	760.97	Joback Method
cpg	598.76	J/mol×K	797.39	Joback Method
cpg	613.00	J/mol×K	833.80	Joback Method
cpg	626.91	J/mol×K	870.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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