(-)-«gamma»-curcumen-15-al

Inchi: InChI=1S/C15H22O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5,7,9,11,13H,4,6,8,10
InchiKey: IAYOZXCTYXYCHP-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC(C)=CCCC(C)C1=CC=C(C=O)CC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	117.95	kJ/mol	Joback Method
hf	-169.08	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1746.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	627.36	K	Joback Method
tc	836.50	K	Joback Method
tf	304.95	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.46	J/mol×K	627.36	Joback Method
cpg	537.27	J/mol×K	662.22	Joback Method
cpg	554.04	J/mol×K	697.07	Joback Method
cpg	569.80	J/mol×K	731.93	Joback Method
cpg	584.62	J/mol×K	766.79	Joback Method
cpg	598.55	J/mol×K	801.64	Joback Method
cpg	611.63	J/mol×K	836.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233404&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