

(Z)-«gamma»-Curcumen-12-yl formate

Inchi:	InChI=1S/C16H24O2/c1-13-7-9-16(10-8-13)15(3)6-4-5-14(2)11-18-12-17/h5,7,9,12,15H,
InchiKey:	DLKFJGNOPMPJPZ-AGKVCYSUSA-N
Formula:	C16H24O2
SMILES:	CC1=CC=C(C(C)CCC=C(C)COC=O)CC1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	21.37	kJ/mol	Joback Method
hf	-321.94	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.189		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1746.00		NIST Webbook
rinpol	1746.00		NIST Webbook
tb	672.66	K	Joback Method
tc	876.81	K	Joback Method
tf	338.45	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.94	J/molxK	672.66	Joback Method
cpg	618.67	J/molxK	706.69	Joback Method
cpg	635.39	J/molxK	740.71	Joback Method
cpg	651.13	J/molxK	774.74	Joback Method
cpg	665.92	J/molxK	808.76	Joback Method
cpg	679.82	J/molxK	842.79	Joback Method
cpg	692.86	J/molxK	876.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R233286&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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