(Z)-«gamma»-Curcumen-12-yl acetate

Inchi: InChI=1S/C17H26O2/c1-13-8-10-17(11-9-13)15(3)7-5-6-14(2)12-19-16(4)18/h6,8,10,15H
InchiKey: YMXKOSQCKRGYRW-XXUROBRHSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CCCC(C)C1=CC=C(C)CC1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	0.39	kJ/mol	Joback Method
hf	-369.58	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	64.89	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.579		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	1808.00		NIST Webbook
tb	700.75	K	Joback Method
tc	906.19	K	Joback Method
tf	357.65	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.28	J/mol×K	700.75	Joback Method
cpg	674.60	J/mol×K	734.99	Joback Method
cpg	691.85	J/mol×K	769.23	Joback Method
cpg	708.08	J/mol×K	803.47	Joback Method
cpg	723.31	J/mol×K	837.71	Joback Method
cpg	737.59	J/mol×K	871.95	Joback Method
cpg	750.97	J/mol×K	906.19	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=R233271&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