Methyl ar-curcumen-12-oate

Inchi: InChI=1S/C16H22O2/c1-12-8-10-15(11-9-12)13(2)6-5-7-14(3)16(17)18-4/h7-11,13H,5-6H
InchiKey: XICYLTQBNRFIHM-AUWJEWJLSA-N
Formula: C16H22O2
SMILES: COC(=O)C(C)=CCCC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	21.93	kJ/mol	Joback Method
hf	-291.16	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.998		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
ripol	2450.00		NIST Webbook
tb	677.03	K	Joback Method
tc	886.86	K	Joback Method
tf	347.14	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.77	J/mol×K	677.03	Joback Method
cpg	594.84	J/mol×K	712.00	Joback Method
cpg	610.90	J/mol×K	746.97	Joback Method
cpg	625.97	J/mol×K	781.95	Joback Method
cpg	640.10	J/mol×K	816.92	Joback Method
cpg	653.34	J/mol×K	851.89	Joback Method
cpg	665.72	J/mol×K	886.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503114&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume