

Y-Curcumenal

Inchi:	InChI=1S/C15H20O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h4-5,7-11,13-14H,6H2,
InchiKey:	STQHHYPRNPVXTF-SNAWJCMRSA-N
Formula:	C15H20O
SMILES:	Cc1ccc(C(C)CC=CC(C)C=O)cc1
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	154.02	kJ/mol	Joback Method
hf	-106.79	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.880		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	626.20	K	Joback Method
tc	837.81	K	Joback Method
tf	304.67	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.42	J/molxK	626.20	Joback Method
cpg	515.34	J/molxK	661.47	Joback Method
cpg	531.21	J/molxK	696.74	Joback Method
cpg	546.10	J/molxK	732.00	Joback Method
cpg	560.06	J/molxK	767.27	Joback Method
cpg	573.15	J/molxK	802.54	Joback Method
cpg	585.42	J/molxK	837.81	Joback Method
dvisc	0.0037370	Paxs	304.67	Joback Method

dvisc	0.0014350	Paxs	358.26	Joback Method
dvisc	0.0007069	Paxs	411.85	Joback Method
dvisc	0.0004099	Paxs	465.44	Joback Method
dvisc	0.0002660	Paxs	519.02	Joback Method
dvisc	0.0001871	Paxs	572.61	Joback Method
dvisc	0.0001398	Paxs	626.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203884&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
dvisc:	Dynamic viscosity
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

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