(E)-Werneria chromene

Inchi: InChI=1S/C15H16O3/c1-15(2)9-8-12-10-11(4-6-13(12)18-15)5-7-14(16)17-3/h4-10H,1-3H
InchiKey: AOZKTJDXDYSFAE-FNORWQNLSA-N
Formula: C15H16O3
SMILES: COC(=O)C=Cc1ccc2c(c1)C=CC(C)(C)O2
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
gf	1.87	kJ/mol	Joback Method
hf	-259.26	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.057		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1985.00		NIST Webbook
tb	697.05	K	Joback Method
tc	931.49	K	Joback Method
tf	443.00	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.47	J/mol×K	697.05	Joback Method
cpg	529.78	J/mol×K	736.12	Joback Method
cpg	544.35	J/mol×K	775.20	Joback Method
cpg	558.35	J/mol×K	814.27	Joback Method
cpg	571.97	J/mol×K	853.34	Joback Method
cpg	585.37	J/mol×K	892.41	Joback Method
cpg	598.73	J/mol×K	931.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519763&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume