Guaiacyl tiglate

Inchi: InChI=1S/C12H14O3/c1-4-9(2)12(13)15-11-8-6-5-7-10(11)14-3/h4-8H,1-3H3/b9-4+
InchiKey: MNXOFCMTJXDHDP-RUDMXATFSA-N
Formula: C12H14O3
SMILES: CC=C(C)C(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 206.24

Physical Properties

Property code	Value	Unit	Source
gf	-114.31	kJ/mol	Joback Method
hf	-335.54	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.567		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
ripol	2333.00		NIST Webbook
tb	608.37	K	Joback Method
tc	825.53	K	Joback Method
tf	339.29	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.54	J/mol×K	608.37	Joback Method
cpg	412.85	J/mol×K	644.56	Joback Method
cpg	426.33	J/mol×K	680.76	Joback Method
cpg	439.00	J/mol×K	716.95	Joback Method
cpg	450.87	J/mol×K	753.14	Joback Method
cpg	461.96	J/mol×K	789.34	Joback Method
cpg	472.29	J/mol×K	825.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383649&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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