

Homogentisic acid, dimethyl ether, methyl ester

Inchi:	InChI=1S/C11H14O4/c1-13-9-4-5-10(14-2)8(6-9)7-11(12)15-3/h4-6H,7H2,1-3H3
InchiKey:	NGFZJWMCFOTWNI-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	<chem>COC(=O)Cc1cc(OC)ccc1OC</chem>
Mol. weight [g/mol]:	210.23

Physical Properties

Property code	Value	Unit	Source
gf	-309.03	kJ/mol	Joback Method
hf	-566.02	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.419		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1616.50		NIST Webbook
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tb	608.85	K	Joback Method
tc	815.75	K	Joback Method
tf	381.81	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.96	J/molxK	608.85	Joback Method
cpg	455.79	J/molxK	781.27	Joback Method
cpg	444.99	J/molxK	746.78	Joback Method
cpg	433.48	J/molxK	712.30	Joback Method
cpg	421.30	J/molxK	677.82	Joback Method
cpg	408.45	J/molxK	643.33	Joback Method
cpg	465.87	J/molxK	815.75	Joback Method
dvisc	0.0001254	Paxs	608.85	Joback Method

dvisc	0.0001540	Paxs	571.01	Joback Method
dvisc	0.0001948	Paxs	533.17	Joback Method
dvisc	0.0002553	Paxs	495.33	Joback Method
dvisc	0.0003500	Paxs	457.49	Joback Method
dvisc	0.0005080	Paxs	419.65	Joback Method
dvisc	0.0007937	Paxs	381.81	Joback Method

Sources

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=U333492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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