

opianic acid

Inchi:	InChI=1S/C10H10O5/c1-14-7-4-3-6(5-11)8(10(12)13)9(7)15-2/h3-5H,1-2H3,(H,12,13)
InchiKey:	HVXXOIGTXJOVON-UHFFFAOYSA-N
Formula:	C10H10O5
SMILES:	COc1ccc(C=O)c(C(=O)O)c1OC
Mol. weight [g/mol]:	210.19

Physical Properties

Property code	Value	Unit	Source
gf	-458.42	kJ/mol	Joback Method
hf	-662.44	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	77.08	kJ/mol	Joback Method
log10ws	-1.92		Aqueous Solubility Prediction Method
logp	1.214		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	709.37	K	Joback Method
tc	911.84	K	Joback Method
tf	421.65	K	Aqueous Solubility Prediction Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.78	J/molxK	709.37	Joback Method
cpg	392.04	J/molxK	743.11	Joback Method
cpg	400.74	J/molxK	776.86	Joback Method
cpg	408.85	J/molxK	810.60	Joback Method
cpg	416.38	J/molxK	844.35	Joback Method
cpg	423.29	J/molxK	878.09	Joback Method
cpg	429.60	J/molxK	911.84	Joback Method
dvisc	0.0006640	Paxs	463.65	Joback Method

dvisc	0.0003576	Paxs	504.60	Joback Method
dvisc	0.0002114	Paxs	545.56	Joback Method
dvisc	0.0001345	Paxs	586.51	Joback Method
dvisc	0.0000908	Paxs	627.46	Joback Method
dvisc	0.0000643	Paxs	668.42	Joback Method
dvisc	0.0000474	Paxs	709.37	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

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