2,4-Dihydroxy-6-(2-oxoheptyl)benzoic acid (Olivetonic acid)

Inchi: InChI=1S/C14H18O5/c1-2-3-4-5-10(15)6-9-7-11(16)8-12(17)13(9)14(18)19/h7-8,16-17H,

InchiKey: DHTUEPZEWVIXGJ-UHFFFAOYSA-N

Formula: C14H18O5

SMILES: CCCCCC(=O)Cc1cc(O)cc(O)c1C(=O)O

Mol. weight [g/mol]: 266.29

Physical Properties

Property code	Value	Unit	Source
gf	-534.12	kJ/mol	Joback Method
hf	-839.24	kJ/mol	Joback Method
hfus	44.52	kJ/mol	Joback Method
hvap	105.90	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.488		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	912.54	K	Joback Method
tc	1131.68	K	Joback Method
tf	670.60	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.54	J/mol×K	912.54	Joback Method
cpg	645.88	J/mol×K	949.06	Joback Method
cpg	657.14	J/mol×K	985.59	Joback Method
cpg	668.44	J/mol×K	1022.11	Joback Method
cpg	679.90	J/mol×K	1058.63	Joback Method
cpg	691.65	J/mol×K	1095.15	Joback Method
cpg	703.81	J/mol×K	1131.68	Joback Method
dvisc	0.0000017	Pa×s	670.60	Joback Method

dvisc	0.0000008	Pa×s	710.92	Joback Method
dvisc	0.0000004	Pa×s	751.25	Joback Method
dvisc	0.0000002	Pa×s	791.57	Joback Method
dvisc	0.0000001	Pa×s	831.89	Joback Method
dvisc	8.1089679e-08	Pa×s	872.22	Joback Method
dvisc	5.1794389e-08	Pa×s	912.54	Joback Method

Sources

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=R627913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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