1-(3,5-Dihydroxyphenyl)heptan-2-one

Inchi: InChI=1S/C13H18O3/c1-2-3-4-5-11(14)6-10-7-12(15)9-13(16)8-10/h7-9,15-16H,2-6H2,1
InchiKey: UYOAKZGQLBHUHR-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCCCCC(=O)Cc1cc(O)cc(O)c1
Mol. weight [g/mol]: 222.28
CAS: 15601-09-9

Physical Properties

Property code	Value	Unit	Source
gf	-267.17	kJ/mol	Joback Method
hf	-542.32	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.790		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	2132.30		NIST Webbook
rinpol	2132.30		NIST Webbook
tb	738.63	K	Joback Method
tc	961.47	K	Joback Method
tf	536.06	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.48	J/mol×K	738.63	Joback Method
cpg	536.25	J/mol×K	775.77	Joback Method
cpg	548.43	J/mol×K	812.91	Joback Method
cpg	560.14	J/mol×K	850.05	Joback Method
cpg	571.51	J/mol×K	887.19	Joback Method
cpg	582.68	J/mol×K	924.33	Joback Method
cpg	593.77	J/mol×K	961.47	Joback Method

dvisc	0.0000410	Pa×s	536.06	Joback Method
dvisc	0.0000193	Pa×s	569.82	Joback Method
dvisc	0.0000098	Pa×s	603.58	Joback Method
dvisc	0.0000054	Pa×s	637.35	Joback Method
dvisc	0.0000031	Pa×s	671.11	Joback Method
dvisc	0.0000019	Pa×s	704.87	Joback Method
dvisc	0.0000012	Pa×s	738.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15601099&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
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