Dihydrodaidzein (keto)

Inchi: InChI=1S/C15H12O4/c16-10-3-1-9(2-4-10)13-8-19-14-7-11(17)5-6-12(14)15(13)18/h1-7,
InchiKey: JHYXBPPMXZIHKG-UHFFFAOYSA-N
Formula: C15H12O4
SMILES: O=C1c2ccc(O)cc2OCC1c1ccc(O)cc1
Mol. weight [g/mol]: 256.25

Physical Properties

Property code	Value	Unit	Source
gf	-178.69	kJ/mol	Joback Method
hf	-449.02	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.457		Crippen Method
mcvol	183.010	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	2666.00		NIST Webbook
tb	867.96	K	Joback Method
tc	1147.06	K	Joback Method
tf	656.82	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.27	J/mol×K	867.96	Joback Method
cpg	573.93	J/mol×K	914.48	Joback Method
cpg	587.16	J/mol×K	960.99	Joback Method
cpg	600.21	J/mol×K	1007.51	Joback Method
cpg	613.33	J/mol×K	1054.03	Joback Method
cpg	626.76	J/mol×K	1100.54	Joback Method
cpg	640.74	J/mol×K	1147.06	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=R261479&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
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