(6aR,12aR)-6a,12a-Dihydro-6H-[1,3]dioxolo[4',5':5,

Inchi: InChI=1S/C16H12O5/c17-8-1-2-9-12(3-8)18-6-11-10-4-14-15(20-7-19-14)5-13(10)21-16(

InchiKey: HUKSJTUUSUGIDC-BDJLRTHQSA-N

Formula: C16H12O5

SMILES: Oc1ccc2c(c1)OCC1c3cc4c(cc3OC21)OCO4

Mol. weight [g/mol]: 284.26

CAS: 2035-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-26.90	kJ/mol	Joback Method
hf	-406.80	kJ/mol	Joback Method
hfus	56.86	kJ/mol	Joback Method
hvap	89.34	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.731		Crippen Method
mcvol	185.550	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	2724.90		NIST Webbook
rinpol	2724.90		NIST Webbook
tb	847.80	K	Joback Method
tc	1112.39	K	Joback Method
tf	652.58	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.69	J/mol×K	847.80	Joback Method
cpg	594.78	J/mol×K	891.90	Joback Method
cpg	607.72	J/mol×K	936.00	Joback Method
cpg	620.81	J/mol×K	980.09	Joback Method
cpg	634.35	J/mol×K	1024.19	Joback Method
cpg	648.64	J/mol×K	1068.29	Joback Method
cpg	663.99	J/mol×K	1112.39	Joback Method

dvisc	0.0006093	Pa×s	652.58	Joback Method
dvisc	0.0004694	Pa×s	685.12	Joback Method
dvisc	0.0003702	Pa×s	717.65	Joback Method
dvisc	0.0002981	Pa×s	750.19	Joback Method
dvisc	0.0002444	Pa×s	782.73	Joback Method
dvisc	0.0002035	Pa×s	815.26	Joback Method
dvisc	0.0001719	Pa×s	847.80	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=C2035156&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