

3,9-dimethoxy-6H,12H-dibenzo[b,f][1,5]dioxocine-

Inchi:	InChI=1S/C16H12O6/c1-19-9-3-5-11-13(7-9)21-16(18)12-6-4-10(20-2)8-14(12)22-15(11)
InchiKey:	JGBUSYJENPDLOQ-UHFFFAOYSA-N
Formula:	C16H12O6
SMILES:	COc1ccc2c(c1)OC(=O)c1ccc(OC)cc1OC2=O
Mol. weight [g/mol]:	300.26

Physical Properties

Property code	Value	Unit	Source
gf	-300.92	kJ/mol	Joback Method
hf	-663.25	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	81.14	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.456		Crippen Method
mvol	204.540	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	888.82	K	Joback Method
tc	1149.83	K	Joback Method
tf	625.70	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.74	J/mol×K	888.82	Joback Method
cpg	629.73	J/mol×K	932.32	Joback Method
cpg	639.89	J/mol×K	975.82	Joback Method
cpg	648.17	J/mol×K	1019.33	Joback Method
cpg	654.51	J/mol×K	1062.83	Joback Method
cpg	658.84	J/mol×K	1106.33	Joback Method
cpg	661.10	J/mol×K	1149.83	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=U374981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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