Phloretin, tetramethyl ether

Other names: 3-(4-Methoxyphenyl)-1-(2,4,6-trimethoxyphenyl)propan-1-one
Inchi: InChI=1S/C19H22O5/c1-21-14-8-5-13(6-9-14)7-10-16(20)19-17(23-3)11-15(22-2)12-18(1
InchiKey: OTGNHTCWPYBYKB-UHFFFAOYSA-N
Formula: C19H22O5
SMILES: COc1ccc(CCC(=O)c2c(OC)cc(OC)cc2OC)cc1
Mol. weight [g/mol]: 330.38

Physical Properties

Property code	Value	Unit	Source
gf	-253.52	kJ/mol	Joback Method
hf	-649.77	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	81.47	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.536		Crippen Method
mcvol	256.100	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	2739.00		NIST Webbook
tb	850.95	K	Joback Method
tc	1070.55	K	Joback Method
tf	545.66	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.54	J/mol×K	850.95	Joback Method
cpg	821.71	J/mol×K	1033.95	Joback Method
cpg	812.66	J/mol×K	997.35	Joback Method
cpg	802.20	J/mol×K	960.75	Joback Method
cpg	790.35	J/mol×K	924.15	Joback Method
cpg	777.12	J/mol×K	887.55	Joback Method
cpg	829.33	J/mol×K	1070.55	Joback Method
dvisc	0.0000394	Pa×s	850.95	Joback Method

dvisc	0.0000482	Pa×s	800.07	Joback Method
dvisc	0.0000606	Pa×s	749.19	Joback Method
dvisc	0.0000788	Pa×s	698.31	Joback Method
dvisc	0.0001067	Pa×s	647.42	Joback Method
dvisc	0.0001521	Pa×s	596.54	Joback Method
dvisc	0.0002319	Pa×s	545.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333706&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