Fumaric acid, 2,6-dimethoxyphenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C23H20O6/c1-26-19-8-5-9-20(27-2)23(19)29-22(25)13-12-21(24)28-15-16-10-

InchiKey: JEDOFCZMQYIACL-OUKQBFOZSA-N

Formula: C23H20O6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 392.40

Physical Properties

Property code	Value	Unit	Source
gf	-152.26	kJ/mol	Joback Method
hf	-525.15	kJ/mol	Joback Method
hfus	47.41	kJ/mol	Joback Method
hvap	98.06	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.062		Crippen Method
mcvol	290.270	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	3209.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	1014.50	K	Joback Method
tc	1256.99	K	Joback Method
tf	655.77	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.60	J/mol×K	1014.50	Joback Method
cpg	934.99	J/mol×K	1216.58	Joback Method
cpg	929.43	J/mol×K	1176.16	Joback Method
cpg	922.66	J/mol×K	1135.75	Joback Method
cpg	914.63	J/mol×K	1095.33	Joback Method
cpg	905.30	J/mol×K	1054.92	Joback Method
cpg	939.40	J/mol×K	1256.99	Joback Method
dvisc	0.0000396	Pa×s	1014.50	Joback Method

dvisc	0.0000478	Pa×s	954.71	Joback Method
dvisc	0.0000591	Pa×s	894.92	Joback Method
dvisc	0.0000754	Pa×s	835.13	Joback Method
dvisc	0.0001000	Pa×s	775.35	Joback Method
dvisc	0.0001388	Pa×s	715.56	Joback Method
dvisc	0.0002047	Pa×s	655.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405764&Units=SI

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