Fumaric acid, 3,4-dimethoxyphenyl isohexyl ester

Inchi: InChI=1S/C18H24O6/c1-13(2)6-5-11-23-17(19)9-10-18(20)24-14-7-8-15(21-3)16(12-14)2

InchiKey: WFFUTSPRGBPXKH-MDZDMXLPSA-N

Formula: C18H24O6

SMILES: COc1ccc(OC(=O)C=CC(=O)OCCCC(C)C)cc1OC

Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-406.23	kJ/mol	Joback Method
hf	-843.36	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.145		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2536.00		NIST Webbook
tb	849.02	K	Joback Method
tc	1057.00	K	Joback Method
tf	512.78	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.61	J/mol×K	849.02	Joback Method
cpg	805.92	J/mol×K	883.68	Joback Method
cpg	819.06	J/mol×K	918.35	Joback Method
cpg	831.02	J/mol×K	953.01	Joback Method
cpg	841.80	J/mol×K	987.67	Joback Method
cpg	851.40	J/mol×K	1022.34	Joback Method
cpg	859.81	J/mol×K	1057.00	Joback Method
dvisc	0.0003185	Pa×s	512.78	Joback Method
dvisc	0.0001814	Pa×s	568.82	Joback Method

dvisc	0.0001143	Pa×s	624.86	Joback Method
dvisc	0.0000777	Pa×s	680.90	Joback Method
dvisc	0.0000560	Pa×s	736.94	Joback Method
dvisc	0.0000423	Pa×s	792.98	Joback Method
dvisc	0.0000331	Pa×s	849.02	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=U348168&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