Fumaric acid, 3,4-dimethoxyphenyl octyl ester

Inchi: InChI=1S/C20H28O6/c1-4-5-6-7-8-9-14-25-19(21)12-13-20(22)26-16-10-11-17(23-2)18(1
InchiKey: CQCGQSYPSYKWFU-OUKQBFOZSA-N
Formula: C20H28O6
SMILES: CCCCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-386.95	kJ/mol	Joback Method
hf	-879.36	kJ/mol	Joback Method
hfus	48.97	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.069		Crippen Method
mcvol	291.220	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	895.22	K	Joback Method
tc	1102.88	K	Joback Method
tf	550.32	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.89	J/mol×K	895.22	Joback Method
cpg	967.91	J/mol×K	1068.27	Joback Method
cpg	958.43	J/mol×K	1033.66	Joback Method
cpg	947.69	J/mol×K	999.05	Joback Method
cpg	935.68	J/mol×K	964.44	Joback Method
cpg	922.42	J/mol×K	929.83	Joback Method
cpg	976.15	J/mol×K	1102.88	Joback Method
dvisc	0.0000273	Pa×s	895.22	Joback Method

dvisc	0.0000345	Pa×s	837.74	Joback Method
dvisc	0.0000453	Pa×s	780.25	Joback Method
dvisc	0.0000620	Pa×s	722.77	Joback Method
dvisc	0.0000896	Pa×s	665.29	Joback Method
dvisc	0.0001389	Pa×s	607.80	Joback Method
dvisc	0.0002359	Pa×s	550.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348171&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