Fumaric acid, 3,4-dimethoxyphenyl tridecyl ester

Inchi: InChI=1S/C25H38O6/c1-4-5-6-7-8-9-10-11-12-13-14-19-30-24(26)17-18-25(27)31-21-15
InchiKey: WLOVWAUMUNMRJE-ISLYRVAYSA-N
Formula: C25H38O6
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 434.57

Physical Properties

Property code	Value	Unit	Source
gf	-344.85	kJ/mol	Joback Method
hf	-982.56	kJ/mol	Joback Method
hfus	61.92	kJ/mol	Joback Method
hvap	97.93	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.020		Crippen Method
mcvol	361.670	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1009.62	K	Joback Method
tc	1236.87	K	Joback Method
tf	606.67	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.10	J/mol×K	1009.62	Joback Method
cpg	1225.32	J/mol×K	1047.49	Joback Method
cpg	1238.80	J/mol×K	1085.37	Joback Method
cpg	1250.55	J/mol×K	1123.24	Joback Method
cpg	1260.60	J/mol×K	1161.12	Joback Method
cpg	1268.97	J/mol×K	1198.99	Joback Method
cpg	1275.69	J/mol×K	1236.87	Joback Method
dvisc	0.0001343	Pa×s	606.67	Joback Method

dvisc	0.0000749	Pa×s	673.83	Joback Method
dvisc	0.0000465	Pa×s	740.99	Joback Method
dvisc	0.0000312	Pa×s	808.14	Joback Method
dvisc	0.0000223	Pa×s	875.30	Joback Method
dvisc	0.0000167	Pa×s	942.46	Joback Method
dvisc	0.0000130	Pa×s	1009.62	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=U348175&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

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