Fumaric acid, 4-methoxyphenyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C23H32O5/c1-3-4-5-6-7-8-9-10-11-12-19-27-22(24)17-18-23(25)28-21-15-13-2

InchiKey: LDYPAJFGYPLSCN-WCPGOBTASA-N

Formula: C23H32O5

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 388.50

Physical Properties

Property code	Value	Unit	Source
gf	-166.84	kJ/mol	Joback Method
hf	-680.37	kJ/mol	Joback Method
hfus	56.14	kJ/mol	Joback Method
hvap	90.37	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.397		Crippen Method
mcvol	323.320	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	940.62	K	Joback Method
tc	1154.42	K	Joback Method
tf	544.30	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.69	J/mol×K	940.62	Joback Method
cpg	1047.12	J/mol×K	976.25	Joback Method
cpg	1061.34	J/mol×K	1011.89	Joback Method
cpg	1074.41	J/mol×K	1047.52	Joback Method
cpg	1086.36	J/mol×K	1083.15	Joback Method
cpg	1097.25	J/mol×K	1118.79	Joback Method
cpg	1107.12	J/mol×K	1154.42	Joback Method
dvisc	0.0002556	Pa×s	544.30	Joback Method

dvisc	0.0001334	Pa×s	610.35	Joback Method
dvisc	0.0000791	Pa×s	676.41	Joback Method
dvisc	0.0000514	Pa×s	742.46	Joback Method
dvisc	0.0000359	Pa×s	808.51	Joback Method
dvisc	0.0000264	Pa×s	874.57	Joback Method
dvisc	0.0000203	Pa×s	940.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405784&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