Fumaric acid, 2-methylphenyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C23H32O4/c1-3-4-5-6-7-8-9-10-11-14-19-26-22(24)17-18-23(25)27-21-16-13-1

InchiKey: SMKDUFRXDKELGB-LWVORGKXSA-N

Formula: C23H32O4

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccccc1C

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-61.84	kJ/mol	Joback Method
hf	-548.15	kJ/mol	Joback Method
hfus	54.96	kJ/mol	Joback Method
hvap	87.96	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.697		Crippen Method
mcvol	317.450	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	918.20	K	Joback Method
tc	1129.38	K	Joback Method
tf	522.07	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.71	J/mol×K	918.20	Joback Method
cpg	1018.71	J/mol×K	953.40	Joback Method
cpg	1033.62	J/mol×K	988.59	Joback Method
cpg	1047.50	J/mol×K	1023.79	Joback Method
cpg	1060.40	J/mol×K	1058.99	Joback Method
cpg	1072.39	J/mol×K	1094.18	Joback Method
cpg	1083.53	J/mol×K	1129.38	Joback Method
dvisc	0.0003684	Pa×s	522.07	Joback Method

dvisc	0.0001873	Pa×s	588.09	Joback Method
dvisc	0.0001091	Pa×s	654.11	Joback Method
dvisc	0.0000702	Pa×s	720.13	Joback Method
dvisc	0.0000486	Pa×s	786.16	Joback Method
dvisc	0.0000357	Pa×s	852.18	Joback Method
dvisc	0.0000273	Pa×s	918.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405690&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