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

Inchi: InChI=1S/C25H36O4/c1-4-5-6-7-8-9-10-11-12-15-20-28-24(26)18-19-25(27)29-23-17-14

InchiKey: BVUIZCVUPIUNBZ-AHSPQICUSA-N

Formula: C25H36O4

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

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-47.44	kJ/mol	Joback Method
hf	-594.71	kJ/mol	Joback Method
hfus	56.61	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.512		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2851.00		NIST Webbook
rinpol	2851.00		NIST Webbook
tb	963.52	K	Joback Method
tc	1181.02	K	Joback Method
tf	529.61	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.25	J/mol×K	963.52	Joback Method
cpg	1141.85	J/mol×K	999.77	Joback Method
cpg	1157.26	J/mol×K	1036.02	Joback Method
cpg	1171.56	J/mol×K	1072.27	Joback Method
cpg	1184.82	J/mol×K	1108.52	Joback Method
cpg	1197.10	J/mol×K	1144.77	Joback Method
cpg	1208.50	J/mol×K	1181.02	Joback Method
dvisc	0.0003274	Pa×s	529.61	Joback Method

dvisc	0.0001523	Pa×s	601.93	Joback Method
dvisc	0.0000835	Pa×s	674.25	Joback Method
dvisc	0.0000514	Pa×s	746.57	Joback Method
dvisc	0.0000345	Pa×s	818.88	Joback Method
dvisc	0.0000247	Pa×s	891.20	Joback Method
dvisc	0.0000186	Pa×s	963.52	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=U405873&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