

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:	CCCCCCCCC=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.25	J/molxK	963.52	Joback Method
cpg	1197.10	J/molxK	1144.77	Joback Method
cpg	1184.82	J/molxK	1108.52	Joback Method
cpg	1171.56	J/molxK	1072.27	Joback Method
cpg	1157.26	J/molxK	1036.02	Joback Method
cpg	1141.85	J/molxK	999.77	Joback Method
cpg	1208.50	J/molxK	1181.02	Joback Method
dvisc	0.0000186	Paxs	963.52	Joback Method

dvisc	0.0000247	Paxs	891.20	Joback Method
dvisc	0.0000345	Paxs	818.88	Joback Method
dvisc	0.0000514	Paxs	746.57	Joback Method
dvisc	0.0000835	Paxs	674.25	Joback Method
dvisc	0.0001523	Paxs	601.93	Joback Method
dvisc	0.0003274	Paxs	529.61	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.chemeo.com/cid/95-291-4/Fumaric-acid-2-isopropylphenyl-dodec-2-en-1-yl-ester.pdf>

Generated by Cheméo on 2025-12-05 09:23:25.056034753 +0000 UTC m=+4674802.586075407.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.