

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

Inchi:	InChI=1S/C23H32O5/c1-3-4-5-6-7-8-9-10-11-14-19-27-22(24)17-18-23(25)28-21-16-13-
InchiKey:	OEROSHYBIVFKBS-LWVORGKXSA-N
Formula:	C23H32O5
SMILES:	CCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccccc1OC
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
mvol	323.320	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	940.62	K	Joback Method
tc	1154.42	K	Joback Method
tf	544.30	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.69	J/molxK	940.62	Joback Method
cpg	1097.25	J/molxK	1118.79	Joback Method
cpg	1086.36	J/molxK	1083.15	Joback Method
cpg	1074.41	J/molxK	1047.52	Joback Method
cpg	1061.34	J/molxK	1011.89	Joback Method
cpg	1047.12	J/molxK	976.25	Joback Method
cpg	1107.12	J/molxK	1154.42	Joback Method
dvisc	0.0000203	Paxs	940.62	Joback Method

dvisc	0.0000264	Paxs	874.57	Joback Method
dvisc	0.0000359	Paxs	808.51	Joback Method
dvisc	0.0000514	Paxs	742.46	Joback Method
dvisc	0.0000791	Paxs	676.41	Joback Method
dvisc	0.0001334	Paxs	610.35	Joback Method
dvisc	0.0002556	Paxs	544.30	Joback Method

Sources

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=U405941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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