Fumaric acid, 2-isopropoxyphenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C24H22O5/c1-17(2)28-21-9-5-6-10-22(21)29-24(26)14-13-23(25)27-16-18-11-

InchiKey: SYWNLBBWUDQTHV-BUHFOSPRSA-N

Formula: C24H22O5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 390.43

Physical Properties

Property code	Value	Unit	Source
gf	-31.65	kJ/mol	Joback Method
hf	-407.38	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	96.83	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	4.832		Crippen Method
mcvol	298.490	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
tb	1009.54	K	Joback Method
tc	1252.90	K	Joback Method
tf	617.29	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.11	J/mol×K	1009.54	Joback Method
cpg	942.15	J/mol×K	1050.10	Joback Method
cpg	952.99	J/mol×K	1090.66	Joback Method
cpg	962.71	J/mol×K	1131.22	Joback Method
cpg	971.40	J/mol×K	1171.78	Joback Method
cpg	979.14	J/mol×K	1212.34	Joback Method
cpg	986.04	J/mol×K	1252.90	Joback Method
dvisc	0.0002884	Pa×s	617.29	Joback Method

dvisc	0.0001781	Pa×s	682.67	Joback Method
dvisc	0.0001196	Pa×s	748.04	Joback Method
dvisc	0.0000856	Pa×s	813.41	Joback Method
dvisc	0.0000644	Pa×s	878.79	Joback Method
dvisc	0.0000504	Pa×s	944.16	Joback Method
dvisc	0.0000407	Pa×s	1009.54	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=U405717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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