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

Inchi: InChI=1S/C22H18O5/c1-25-19-8-4-5-9-20(19)27-22(24)13-12-21(23)26-15-16-10-11-17-

InchiKey: IKHZOAPDBMCNCD-OUKQBFOZSA-N

Formula: C22H18O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 362.38

Physical Properties

Property code	Value	Unit	Source
gf	-46.05	kJ/mol	Joback Method
hf	-360.82	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	92.76	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.053		Crippen Method
mcvol	270.310	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	3077.00		NIST Webbook
rinpol	3077.00		NIST Webbook
tb	964.22	K	Joback Method
tc	1207.66	K	Joback Method
tf	609.75	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.95	J/mol×K	964.22	Joback Method
cpg	824.70	J/mol×K	1004.79	Joback Method
cpg	835.28	J/mol×K	1045.37	Joback Method
cpg	844.77	J/mol×K	1085.94	Joback Method
cpg	853.25	J/mol×K	1126.51	Joback Method
cpg	860.80	J/mol×K	1167.09	Joback Method
cpg	867.50	J/mol×K	1207.66	Joback Method
dvisc	0.0003347	Pa×s	609.75	Joback Method

dvisc	0.0002204	Pa×s	668.83	Joback Method
dvisc	0.0001554	Pa×s	727.91	Joback Method
dvisc	0.0001154	Pa×s	786.99	Joback Method
dvisc	0.0000893	Pa×s	846.06	Joback Method
dvisc	0.0000715	Pa×s	905.14	Joback Method
dvisc	0.0000588	Pa×s	964.22	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=U405943&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