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

Inchi: InChI=1S/C22H18O4/c1-16-6-2-5-9-20(16)26-22(24)13-12-21(23)25-15-17-10-11-18-7-3

InchiKey: SQDLOEHYLAICFF-OUKQBFOZSA-N

Formula: C22H18O4

SMILES: Cc1ccccc1OC(=O)C=CC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
gf	58.95	kJ/mol	Joback Method
hf	-228.60	kJ/mol	Joback Method
hfus	42.84	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.353		Crippen Method
mcvol	264.440	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2971.00		NIST Webbook
rinpol	2971.00		NIST Webbook
tb	941.80	K	Joback Method
tc	1186.77	K	Joback Method
tf	587.52	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.27	J/mol×K	941.80	Joback Method
cpg	799.85	J/mol×K	982.63	Joback Method
cpg	811.37	J/mol×K	1023.46	Joback Method
cpg	821.93	J/mol×K	1064.29	Joback Method
cpg	831.64	J/mol×K	1105.12	Joback Method
cpg	840.60	J/mol×K	1145.94	Joback Method
cpg	848.92	J/mol×K	1186.77	Joback Method
dvisc	0.0004573	Pa×s	587.52	Joback Method

dvisc	0.0002977	Pa×s	646.57	Joback Method
dvisc	0.0002082	Pa×s	705.61	Joback Method
dvisc	0.0001539	Pa×s	764.66	Joback Method
dvisc	0.0001188	Pa×s	823.71	Joback Method
dvisc	0.0000950	Pa×s	882.75	Joback Method
dvisc	0.0000780	Pa×s	941.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405691&Units=SI
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

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