Fumaric acid, 1-phenylprop-1-yl naphth-2-ylmethyl ester

Inchi: InChI=1S/C24H22O4/c1-2-22(20-9-4-3-5-10-20)28-24(26)15-14-23(25)27-17-18-12-13-1

InchiKey: NESIGXKNEXPZHS-CCEZHUSRSA-N

Formula: C24H22O4

SMILES: CCC(OC(=O)C=CC(=O)OCc1ccc2ccccc2c1)c1ccccc1

Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	82.98	kJ/mol	Joback Method
hf	-263.69	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	93.75	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.134		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	3072.00		NIST Webbook
rinpol	3072.00		NIST Webbook
tb	982.14	K	Joback Method
tc	1225.18	K	Joback Method
tf	582.54	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.70	J/mol×K	982.14	Joback Method
cpg	918.84	J/mol×K	1022.65	Joback Method
cpg	930.93	J/mol×K	1063.15	Joback Method
cpg	942.10	J/mol×K	1103.66	Joback Method
cpg	952.46	J/mol×K	1144.17	Joback Method
cpg	962.14	J/mol×K	1184.67	Joback Method
cpg	971.24	J/mol×K	1225.18	Joback Method
dvisc	0.0004430	Pa×s	582.54	Joback Method

dvisc	0.0002594	Pa×s	649.14	Joback Method
dvisc	0.0001678	Pa×s	715.74	Joback Method
dvisc	0.0001169	Pa×s	782.34	Joback Method
dvisc	0.0000862	Pa×s	848.94	Joback Method
dvisc	0.0000664	Pa×s	915.54	Joback Method
dvisc	0.0000530	Pa×s	982.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405907&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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