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

Inchi: InChI=1S/C24H22O4/c1-17(2)21-9-5-6-10-22(21)28-24(26)14-13-23(25)27-16-18-11-12-

InchiKey: UDGUBLBQFRVFND-BUHFOSPRSA-N

Formula: C24H22O4

SMILES: CC(C)c1ccccc1OC(=O)C=CC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	73.35	kJ/mol	Joback Method
hf	-275.16	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.168		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		NIST Webbook
tb	987.12	K	Joback Method
tc	1230.90	K	Joback Method
tf	595.06	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.34	J/mol×K	987.12	Joback Method
cpg	917.37	J/mol×K	1027.75	Joback Method
cpg	929.33	J/mol×K	1068.38	Joback Method
cpg	940.34	J/mol×K	1109.01	Joback Method
cpg	950.49	J/mol×K	1149.64	Joback Method
cpg	959.92	J/mol×K	1190.27	Joback Method
cpg	968.71	J/mol×K	1230.90	Joback Method
dvisc	0.0004001	Pa×s	595.06	Joback Method

dvisc	0.0002435	Pa×s	660.40	Joback Method
dvisc	0.0001620	Pa×s	725.75	Joback Method
dvisc	0.0001153	Pa×s	791.09	Joback Method
dvisc	0.0000864	Pa×s	856.43	Joback Method
dvisc	0.0000675	Pa×s	921.78	Joback Method
dvisc	0.0000545	Pa×s	987.12	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=U405874&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