Fumaric acid, di(2-propylphenyl) ester

Inchi: InChI=1S/C22H24O4/c1-3-9-17-11-5-7-13-19(17)25-21(23)15-16-22(24)26-20-14-8-6-12
InchiKey: RICHKLPZEZIMAK-FOCLMDBBSA-N
Formula: C22H24O4
SMILES: CCCc1ccccc1OC(=O)C=CC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-47.70	kJ/mol	Joback Method
hf	-419.67	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	88.71	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.659		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	922.82	K	Joback Method
tc	1150.24	K	Joback Method
tf	554.82	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.60	J/mol×K	922.82	Joback Method
cpg	882.53	J/mol×K	960.72	Joback Method
cpg	895.22	J/mol×K	998.63	Joback Method
cpg	906.72	J/mol×K	1036.53	Joback Method
cpg	917.10	J/mol×K	1074.43	Joback Method
cpg	926.40	J/mol×K	1112.34	Joback Method
cpg	934.69	J/mol×K	1150.24	Joback Method
dvisc	0.0003417	Pa×s	554.82	Joback Method

dvisc	0.0001974	Pa×s	616.15	Joback Method
dvisc	0.0001259	Pa×s	677.49	Joback Method
dvisc	0.0000866	Pa×s	738.82	Joback Method
dvisc	0.0000630	Pa×s	800.15	Joback Method
dvisc	0.0000480	Pa×s	861.49	Joback Method
dvisc	0.0000379	Pa×s	922.82	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=U348130&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