Fumaric acid, hexyl 4-phenylphenyl ester

Inchi: InChI=1S/C22H24O4/c1-2-3-4-8-17-25-21(23)15-16-22(24)26-20-13-11-19(12-14-20)18-
InchiKey: AYHJKGZICXWMLZ-FOCLMDBBSA-N
Formula: C22H24O4
SMILES: CCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-38.07	kJ/mol	Joback Method
hf	-408.20	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	88.05	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.939		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	917.84	K	Joback Method
tc	1144.48	K	Joback Method
tf	542.30	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.75	J/mol×K	917.84	Joback Method
cpg	928.26	J/mol×K	1106.71	Joback Method
cpg	918.75	J/mol×K	1068.93	Joback Method
cpg	908.21	J/mol×K	1031.16	Joback Method
cpg	896.58	J/mol×K	993.39	Joback Method
cpg	883.77	J/mol×K	955.61	Joback Method
cpg	936.79	J/mol×K	1144.48	Joback Method
dvisc	0.0000372	Pa×s	917.84	Joback Method

dvisc	0.0000476	Pa×s	855.25	Joback Method
dvisc	0.0000635	Pa×s	792.66	Joback Method
dvisc	0.0000888	Pa×s	730.07	Joback Method
dvisc	0.0001324	Pa×s	667.48	Joback Method
dvisc	0.0002145	Pa×s	604.89	Joback Method
dvisc	0.0003883	Pa×s	542.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348212&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