Fumaric acid, heptyl 4-phenylphenyl ester

Inchi: InChI=1S/C23H26O4/c1-2-3-4-5-9-18-26-22(24)16-17-23(25)27-21-14-12-20(13-15-21)1
InchiKey: NOFHNUOQLIPSML-WUKNDPDISA-N
Formula: C23H26O4
SMILES: CCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-29.65	kJ/mol	Joback Method
hf	-428.84	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.329		Crippen Method
mcvol	297.990	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	3073.00		NIST Webbook
rinpol	3073.00		NIST Webbook
tb	940.72	K	Joback Method
tc	1166.83	K	Joback Method
tf	553.57	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.62	J/mol×K	940.72	Joback Method
cpg	987.57	J/mol×K	1129.15	Joback Method
cpg	977.99	J/mol×K	1091.46	Joback Method
cpg	967.37	J/mol×K	1053.78	Joback Method
cpg	955.64	J/mol×K	1016.09	Joback Method
cpg	942.75	J/mol×K	978.41	Joback Method
cpg	996.18	J/mol×K	1166.83	Joback Method
dvisc	0.0000322	Pa×s	940.72	Joback Method

dvisc	0.0000414	Pa×s	876.20	Joback Method
dvisc	0.0000554	Pa×s	811.67	Joback Method
dvisc	0.0000779	Pa×s	747.14	Joback Method
dvisc	0.0001168	Pa×s	682.62	Joback Method
dvisc	0.0001907	Pa×s	618.09	Joback Method
dvisc	0.0003490	Pa×s	553.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348213&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