Fumaric acid, nonyl 4-phenylphenyl ester

Inchi: InChI=1S/C25H30O4/c1-2-3-4-5-6-7-11-20-28-24(26)18-19-25(27)29-23-16-14-22(15-17
InchiKey: OVAZBVUBJUFZEK-VHEBQXMUSA-N
Formula: C25H30O4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 394.50

Physical Properties

Property code	Value	Unit	Source
gf	-12.81	kJ/mol	Joback Method
hf	-470.12	kJ/mol	Joback Method
hfus	53.97	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.109		Crippen Method
mcvol	326.170	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook
tb	986.48	K	Joback Method
tc	1214.03	K	Joback Method
tf	576.11	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.20	J/mol×K	986.48	Joback Method
cpg	1108.03	J/mol×K	1176.10	Joback Method
cpg	1098.30	J/mol×K	1138.18	Joback Method
cpg	1087.54	J/mol×K	1100.25	Joback Method
cpg	1075.65	J/mol×K	1062.33	Joback Method
cpg	1062.56	J/mol×K	1024.40	Joback Method
cpg	1116.78	J/mol×K	1214.03	Joback Method
dvisc	0.0000241	Pa×s	986.48	Joback Method

dvisc	0.0000311	Pa×s	918.09	Joback Method
dvisc	0.0000419	Pa×s	849.69	Joback Method
dvisc	0.0000594	Pa×s	781.30	Joback Method
dvisc	0.0000901	Pa×s	712.90	Joback Method
dvisc	0.0001494	Pa×s	644.50	Joback Method
dvisc	0.0002790	Pa×s	576.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348215&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