Fumaric acid, isohexyl 4-phenylphenyl ester

Inchi: InChI=1S/C22H24O4/c1-17(2)7-6-16-25-21(23)14-15-22(24)26-20-12-10-19(11-13-20)18
InchiKey: LHWPMEHTNAVVFY-CCEZHUSRSA-N
Formula: C22H24O4
SMILES: CC(C)CCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-40.51	kJ/mol	Joback Method
hf	-413.48	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	87.66	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.795		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2899.00		NIST Webbook
rinpol	2899.00		NIST Webbook
tb	917.40	K	Joback Method
tc	1146.55	K	Joback Method
tf	527.30	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.25	J/mol×K	917.40	Joback Method
cpg	884.38	J/mol×K	955.59	Joback Method
cpg	897.25	J/mol×K	993.78	Joback Method
cpg	908.92	J/mol×K	1031.98	Joback Method
cpg	919.46	J/mol×K	1070.17	Joback Method
cpg	928.92	J/mol×K	1108.36	Joback Method
cpg	937.38	J/mol×K	1146.55	Joback Method
dvisc	0.0004295	Pa×s	527.30	Joback Method

dvisc	0.0002230	Pa×s	592.32	Joback Method
dvisc	0.0001318	Pa×s	657.33	Joback Method
dvisc	0.0000857	Pa×s	722.35	Joback Method
dvisc	0.0000598	Pa×s	787.37	Joback Method
dvisc	0.0000441	Pa×s	852.38	Joback Method
dvisc	0.0000339	Pa×s	917.40	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=U348211&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