Fumaric acid, decyl 4-phenylphenyl ester

Inchi: InChI=1S/C26H32O4/c1-2-3-4-5-6-7-8-12-21-29-25(27)19-20-26(28)30-24-17-15-23(16-1
InchiKey: QYQSXEJQQIPHLI-FMQUCBEESA-N
Formula: C26H32O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	-4.39	kJ/mol	Joback Method
hf	-490.76	kJ/mol	Joback Method
hfus	56.56	kJ/mol	Joback Method
hvap	96.95	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.499		Crippen Method
mcvol	340.260	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	3391.00		NIST Webbook
rinpol	3391.00		NIST Webbook
tb	1009.36	K	Joback Method
tc	1238.98	K	Joback Method
tf	587.38	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.81	J/mol×K	1009.36	Joback Method
cpg	1123.31	J/mol×K	1047.63	Joback Method
cpg	1136.51	J/mol×K	1085.90	Joback Method
cpg	1148.50	J/mol×K	1124.17	Joback Method
cpg	1159.35	J/mol×K	1162.44	Joback Method
cpg	1169.14	J/mol×K	1200.71	Joback Method
cpg	1177.97	J/mol×K	1238.98	Joback Method
dvisc	0.0002483	Pa×s	587.38	Joback Method

dvisc	0.0001316	Pa×s	657.71	Joback Method
dvisc	0.0000789	Pa×s	728.04	Joback Method
dvisc	0.0000517	Pa×s	798.37	Joback Method
dvisc	0.0000363	Pa×s	868.70	Joback Method
dvisc	0.0000269	Pa×s	939.03	Joback Method
dvisc	0.0000208	Pa×s	1009.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348216&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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