Fumaric acid, dodecyl 4-phenylphenyl ester

Inchi: InChI=1S/C28H36O4/c1-2-3-4-5-6-7-8-9-10-14-23-31-27(29)21-22-28(30)32-26-19-17-25
InchiKey: VKJFZZMMKRBKKM-QURGRASLSA-N
Formula: C28H36O4
SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 436.58

Physical Properties

Property code	Value	Unit	Source
gf	12.45	kJ/mol	Joback Method
hf	-532.04	kJ/mol	Joback Method
hfus	61.74	kJ/mol	Joback Method
hvap	101.41	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	7.279		Crippen Method
mcvol	368.440	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3616.00		NIST Webbook
rinpol	3616.00		NIST Webbook
tb	1055.12	K	Joback Method
tc	1291.87	K	Joback Method
tf	609.92	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1231.48	J/mol×K	1055.12	Joback Method
cpg	1293.09	J/mol×K	1252.42	Joback Method
cpg	1283.11	J/mol×K	1212.96	Joback Method
cpg	1272.06	J/mol×K	1173.50	Joback Method
cpg	1259.84	J/mol×K	1134.04	Joback Method
cpg	1246.35	J/mol×K	1094.58	Joback Method
cpg	1302.10	J/mol×K	1291.87	Joback Method
dvisc	0.0000153	Pa×s	1055.12	Joback Method

dvisc	0.0000200	Pa×s	980.92	Joback Method
dvisc	0.0000271	Pa×s	906.72	Joback Method
dvisc	0.0000389	Pa×s	832.52	Joback Method
dvisc	0.0000599	Pa×s	758.32	Joback Method
dvisc	0.0001014	Pa×s	684.12	Joback Method
dvisc	0.0001949	Pa×s	609.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348218&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