Fumaric acid, octyl 4-phenylphenyl ester

Inchi: InChI=1S/C24H28O4/c1-2-3-4-5-6-10-19-27-23(25)17-18-24(26)28-22-15-13-21(14-16-2
InchiKey: QLZHLASOKWEOFJ-ISLYRVAYSA-N
Formula: C24H28O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-21.23	kJ/mol	Joback Method
hf	-449.48	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	92.50	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.719		Crippen Method
mcvol	312.080	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	3176.00		NIST Webbook
rinpol	3176.00		NIST Webbook
tb	963.60	K	Joback Method
tc	1190.00	K	Joback Method
tf	564.84	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.12	J/mol×K	963.60	Joback Method
cpg	1002.36	J/mol×K	1001.33	Joback Method
cpg	1015.35	J/mol×K	1039.07	Joback Method
cpg	1027.15	J/mol×K	1076.80	Joback Method
cpg	1037.85	J/mol×K	1114.53	Joback Method
cpg	1047.50	J/mol×K	1152.26	Joback Method
cpg	1056.19	J/mol×K	1190.00	Joback Method
dvisc	0.0003126	Pa×s	564.84	Joback Method

dvisc	0.0001690	Pa×s	631.30	Joback Method
dvisc	0.0001028	Pa×s	697.76	Joback Method
dvisc	0.0000681	Pa×s	764.22	Joback Method
dvisc	0.0000482	Pa×s	830.68	Joback Method
dvisc	0.0000359	Pa×s	897.14	Joback Method
dvisc	0.0000279	Pa×s	963.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348214&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