Fumaric acid, butyl 4-phenylphenyl ester

Inchi: InChI=1S/C20H20O4/c1-2-3-15-23-19(21)13-14-20(22)24-18-11-9-17(10-12-18)16-7-5-4
InchiKey: KYBLIMZAEQYWIQ-BUHFOSPRSA-N
Formula: C20H20O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-54.91	kJ/mol	Joback Method
hf	-366.92	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	83.60	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.158		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2726.00		NIST Webbook
rinpol	2726.00		NIST Webbook
tb	872.08	K	Joback Method
tc	1102.04	K	Joback Method
tf	519.76	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.10	J/mol×K	872.08	Joback Method
cpg	811.53	J/mol×K	1063.71	Joback Method
cpg	802.24	J/mol×K	1025.39	Joback Method
cpg	791.90	J/mol×K	987.06	Joback Method
cpg	780.48	J/mol×K	948.73	Joback Method
cpg	767.90	J/mol×K	910.41	Joback Method
cpg	819.85	J/mol×K	1102.04	Joback Method
dvisc	0.0000490	Pa×s	872.08	Joback Method

dvisc	0.0000624	Pa×s	813.36	Joback Method
dvisc	0.0000826	Pa×s	754.64	Joback Method
dvisc	0.0001145	Pa×s	695.92	Joback Method
dvisc	0.0001685	Pa×s	637.20	Joback Method
dvisc	0.0002684	Pa×s	578.48	Joback Method
dvisc	0.0004750	Pa×s	519.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348209&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