Fumaric acid, di(3-ethylphenyl) ester

Inchi: InChI=1S/C20H20O4/c1-3-15-7-5-9-17(13-15)23-19(21)11-12-20(22)24-18-10-6-8-16(4-2
InchiKey: SGPKQMANPYGMQT-VAWYXSNFSA-N
Formula: C20H20O4
SMILES: CCc1cccc(OC(=O)C=CC(=O)Oc2cccc(CC)c2)c1
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-64.54	kJ/mol	Joback Method
hf	-378.39	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.879		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	877.06	K	Joback Method
tc	1107.75	K	Joback Method
tf	532.28	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.87	J/mol×K	877.06	Joback Method
cpg	766.57	J/mol×K	915.51	Joback Method
cpg	779.05	J/mol×K	953.96	Joback Method
cpg	790.37	J/mol×K	992.41	Joback Method
cpg	800.57	J/mol×K	1030.85	Joback Method
cpg	809.71	J/mol×K	1069.30	Joback Method
cpg	817.84	J/mol×K	1107.75	Joback Method
dvisc	0.0004152	Pa×s	532.28	Joback Method

dvisc	0.0002455	Pa×s	589.74	Joback Method
dvisc	0.0001593	Pa×s	647.21	Joback Method
dvisc	0.0001110	Pa×s	704.67	Joback Method
dvisc	0.0000816	Pa×s	762.13	Joback Method
dvisc	0.0000627	Pa×s	819.60	Joback Method
dvisc	0.0000498	Pa×s	877.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348161&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