Fumaric acid, di(2,3-dimethylphenyl) ester

Inchi: InChI=1S/C20H20O4/c1-13-7-5-9-17(15(13)3)23-19(21)11-12-20(22)24-18-10-6-8-14(2)1
InchiKey: CSQSWVWAKAKXKA-VAWYXSNFSA-N
Formula: C20H20O4
SMILES: Cc1cccc(OC(=O)C=CC(=O)Oc2cccc(C)c2C)c1C
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-83.80	kJ/mol	Joback Method
hf	-401.33	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	85.58	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	3.987		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	887.02	K	Joback Method
tc	1119.18	K	Joback Method
tf	557.32	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.35	J/mol×K	887.02	Joback Method
cpg	805.95	J/mol×K	1080.49	Joback Method
cpg	797.16	J/mol×K	1041.79	Joback Method
cpg	787.23	J/mol×K	1003.10	Joback Method
cpg	776.15	J/mol×K	964.41	Joback Method
cpg	763.87	J/mol×K	925.71	Joback Method
cpg	813.66	J/mol×K	1119.18	Joback Method
dvisc	0.0000516	Pa×s	887.02	Joback Method

dvisc	0.0000635	Pa×s	832.07	Joback Method
dvisc	0.0000803	Pa×s	777.12	Joback Method
dvisc	0.0001053	Pa×s	722.17	Joback Method
dvisc	0.0001444	Pa×s	667.22	Joback Method
dvisc	0.0002095	Pa×s	612.27	Joback Method
dvisc	0.0003272	Pa×s	557.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348148&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