Fumaric acid, 2-methoxyphenyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H13ClO5/c1-21-14-7-2-3-8-15(14)23-17(20)10-9-16(19)22-13-6-4-5-12(18)

InchiKey: QHDKTLRSSROPPF-MDZDMXLPSA-N

Formula: C17H13ClO5

SMILES: COc1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 332.74

Physical Properties

Property code	Value	Unit	Source
gf	-206.73	kJ/mol	Joback Method
hf	-464.43	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.416		Crippen Method
mcvol	231.560	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	868.27	K	Joback Method
tc	1108.40	K	Joback Method
tf	550.62	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.22	J/mol×K	868.27	Joback Method
cpg	676.16	J/mol×K	1068.38	Joback Method
cpg	669.73	J/mol×K	1028.36	Joback Method
cpg	662.14	J/mol×K	988.34	Joback Method
cpg	653.38	J/mol×K	948.31	Joback Method
cpg	643.41	J/mol×K	908.29	Joback Method
cpg	681.48	J/mol×K	1108.40	Joback Method
dvisc	0.0000492	Pa×s	868.27	Joback Method

dvisc	0.0000611	Pa×s	815.33	Joback Method
dvisc	0.0000781	Pa×s	762.39	Joback Method
dvisc	0.0001035	Pa×s	709.44	Joback Method
dvisc	0.0001436	Pa×s	656.50	Joback Method
dvisc	0.0002111	Pa×s	603.56	Joback Method
dvisc	0.0003341	Pa×s	550.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405937&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

Latest version available from:
https://www.chemeo.com/cid/74-468-1/Fumaric-acid-2-methoxyphenyl-3-chlorophenyl-ester.pdf
Generated by Cheméo on 2024-04-29 07:22:29.102626197 +0000 UTC m=+16664598.023203509.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.