Fumaric acid, 2-methoxyphenyl 8-chlorooctyl ester

Inchi: InChI=1S/C19H25ClO5/c1-23-16-10-6-7-11-17(16)25-19(22)13-12-18(21)24-15-9-5-3-2-4

InchiKey: GKFQEYOXOAHOOY-OUKQBFOZSA-N

Formula: C19H25ClO5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OCCCCCCCCCCl

Mol. weight [g/mol]: 368.85

Physical Properties

Property code	Value	Unit	Source
gf	-292.67	kJ/mol	Joback Method
hf	-730.77	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	85.89	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.279		Crippen Method
mcvol	283.500	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	882.37	K	Joback Method
tc	1091.85	K	Joback Method
tf	534.22	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.19	J/mol×K	882.37	Joback Method
cpg	860.98	J/mol×K	917.28	Joback Method
cpg	873.66	J/mol×K	952.20	Joback Method
cpg	885.22	J/mol×K	987.11	Joback Method
cpg	895.71	J/mol×K	1022.03	Joback Method
cpg	905.14	J/mol×K	1056.94	Joback Method
cpg	913.54	J/mol×K	1091.85	Joback Method
dvisc	0.0003483	Pa×s	534.22	Joback Method

dvisc	0.0001977	Pa×s	592.25	Joback Method
dvisc	0.0001241	Pa×s	650.27	Joback Method
dvisc	0.0000841	Pa×s	708.29	Joback Method
dvisc	0.0000605	Pa×s	766.32	Joback Method
dvisc	0.0000455	Pa×s	824.34	Joback Method
dvisc	0.0000356	Pa×s	882.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405939&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