Fumaric acid, 2-methylphenyl 8-chlorooctyl ester

Inchi: InChI=1S/C19H25ClO4/c1-16-10-6-7-11-17(16)24-19(22)13-12-18(21)23-15-9-5-3-2-4-8-

InchiKey: WYVTYMQROJTVCV-OUKQBFOZSA-N

Formula: C19H25ClO4

SMILES: Cc1ccccc1OC(=O)C=CC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-187.67	kJ/mol	Joback Method
hf	-598.55	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.579		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	859.95	K	Joback Method
tc	1068.62	K	Joback Method
tf	511.99	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.34	J/mol×K	859.95	Joback Method
cpg	833.64	J/mol×K	894.73	Joback Method
cpg	846.90	J/mol×K	929.51	Joback Method
cpg	859.15	J/mol×K	964.29	Joback Method
cpg	870.43	J/mol×K	999.06	Joback Method
cpg	880.77	J/mol×K	1033.84	Joback Method
cpg	890.22	J/mol×K	1068.62	Joback Method
dvisc	0.0004963	Pa×s	511.99	Joback Method

dvisc	0.0002753	Pa×s	569.98	Joback Method
dvisc	0.0001703	Pa×s	627.98	Joback Method
dvisc	0.0001142	Pa×s	685.97	Joback Method
dvisc	0.0000815	Pa×s	743.96	Joback Method
dvisc	0.0000611	Pa×s	801.96	Joback Method
dvisc	0.0000476	Pa×s	859.95	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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