

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:	<chem>Cc1ccccc1OC(=O)C=CC(=O)OCCCCCCCCCI</chem>
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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002753	Paxs	569.98	Joback Method
dvisc	0.0001703	Paxs	627.98	Joback Method
dvisc	0.0001142	Paxs	685.97	Joback Method
dvisc	0.0000815	Paxs	743.96	Joback Method
dvisc	0.0000611	Paxs	801.96	Joback Method
dvisc	0.0000476	Paxs	859.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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