Fumaric acid, 2-(2-methoxyethyl)hexyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C19H23Cl3O5/c1-3-4-5-13(8-9-25-2)12-26-17(23)6-7-18(24)27-19-15(21)10-14

InchiKey: WNUNXUOWHNEZNW-VOTSOKGWSA-N

Formula: C19H23Cl3O5

SMILES: CCCCC(CCOC)COC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 437.74

Physical Properties

Property code	Value	Unit	Source
gf	-338.23	kJ/mol	Joback Method
hf	-790.47	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	95.60	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.494		Crippen Method
mcvol	307.980	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2787.00		NIST Webbook
tb	966.75	K	Joback Method
tc	1190.15	K	Joback Method
tf	604.10	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.14	J/mol×K	966.75	Joback Method
cpg	901.36	J/mol×K	1003.98	Joback Method
cpg	911.34	J/mol×K	1041.22	Joback Method
cpg	920.10	J/mol×K	1078.45	Joback Method
cpg	927.66	J/mol×K	1115.69	Joback Method
cpg	934.05	J/mol×K	1152.92	Joback Method
cpg	939.26	J/mol×K	1190.15	Joback Method
dvisc	0.0001967	Pa×s	604.10	Joback Method
dvisc	0.0001185	Pa×s	664.54	Joback Method

dvisc	0.0000777	Pa×s	724.98	Joback Method
dvisc	0.0000544	Pa×s	785.42	Joback Method
dvisc	0.0000400	Pa×s	845.87	Joback Method
dvisc	0.0000307	Pa×s	906.31	Joback Method
dvisc	0.0000243	Pa×s	966.75	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U405894&Units=SI

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