Fumaric acid, decyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C20H25Cl3O4/c1-2-3-4-5-6-7-8-9-12-26-18(24)10-11-19(25)27-17-14-15(21)13
InchiKey: LWPBKWZRDHPSKM-ZHACJKMWSA-N
Formula: C20H25Cl3O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	-222.37	kJ/mol	Joback Method
hf	-673.61	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.792		Crippen Method
mcvol	316.200	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	967.65	K	Joback Method
tc	1189.54	K	Joback Method
tf	608.14	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.06	J/mol×K	967.65	Joback Method
cpg	934.23	J/mol×K	1004.63	Joback Method
cpg	945.29	J/mol×K	1041.61	Joback Method
cpg	955.28	J/mol×K	1078.60	Joback Method
cpg	964.23	J/mol×K	1115.58	Joback Method
cpg	972.20	J/mol×K	1152.56	Joback Method
cpg	979.20	J/mol×K	1189.54	Joback Method
dvisc	0.0002335	Pa×s	608.14	Joback Method

dvisc	0.0001435	Pa×s	668.06	Joback Method
dvisc	0.0000956	Pa×s	727.98	Joback Method
dvisc	0.0000677	Pa×s	787.89	Joback Method
dvisc	0.0000504	Pa×s	847.81	Joback Method
dvisc	0.0000389	Pa×s	907.73	Joback Method
dvisc	0.0000311	Pa×s	967.65	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=U348291&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