Fumaric acid, pentadecyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C25H35Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-31-23(29)15-16-24(30)32
InchiKey: YGMVWIAHCKPRDU-FOCLMDBBSA-N
Formula: C25H35Cl3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 505.90

Physical Properties

Property code	Value	Unit	Source
gf	-180.27	kJ/mol	Joback Method
hf	-776.81	kJ/mol	Joback Method
hfus	71.75	kJ/mol	Joback Method
hvap	106.93	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.743		Crippen Method
mcvol	386.650	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	3436.00		NIST Webbook
tb	1082.05	K	Joback Method
tc	1326.92	K	Joback Method
tf	664.49	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.50	J/mol×K	1082.05	Joback Method
cpg	1276.27	J/mol×K	1286.11	Joback Method
cpg	1268.10	J/mol×K	1245.30	Joback Method
cpg	1258.71	J/mol×K	1204.49	Joback Method
cpg	1248.03	J/mol×K	1163.67	Joback Method
cpg	1235.99	J/mol×K	1122.86	Joback Method
cpg	1283.30	J/mol×K	1326.92	Joback Method
dvisc	0.0000144	Pa×s	1082.05	Joback Method
dvisc	0.0000183	Pa×s	1012.46	Joback Method

dvisc	0.0000241	Pa×s	942.86	Joback Method
dvisc	0.0000331	Pa×s	873.27	Joback Method
dvisc	0.0000481	Pa×s	803.68	Joback Method
dvisc	0.0000750	Pa×s	734.08	Joback Method
dvisc	0.0001285	Pa×s	664.49	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=U348278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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