Fumaric acid, pentyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C15H15Cl3O4/c1-2-3-4-9-21-12(19)7-8-13(20)22-15-11(17)6-5-10(16)14(15)18

InchiKey: XANIAYLQQMRBCA-BQYQJAHWSA-N

Formula: C15H15Cl3O4

SMILES: CCCCCOC(=O)C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-264.47	kJ/mol	Joback Method
hf	-570.41	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.842		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2464.00		NIST Webbook
tb	853.25	K	Joback Method
tc	1075.15	K	Joback Method
tf	551.79	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.32	J/mol×K	853.25	Joback Method
cpg	648.11	J/mol×K	890.23	Joback Method
cpg	657.98	J/mol×K	927.22	Joback Method
cpg	666.96	J/mol×K	964.20	Joback Method
cpg	675.06	J/mol×K	1001.18	Joback Method
cpg	682.30	J/mol×K	1038.17	Joback Method
cpg	688.71	J/mol×K	1075.15	Joback Method
dvisc	0.0003929	Pa×s	551.79	Joback Method
dvisc	0.0002561	Pa×s	602.03	Joback Method

dvisc	0.0001783	Pa×s	652.28	Joback Method
dvisc	0.0001308	Pa×s	702.52	Joback Method
dvisc	0.0000999	Pa×s	752.76	Joback Method
dvisc	0.0000790	Pa×s	803.01	Joback Method
dvisc	0.0000642	Pa×s	853.25	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=U348223&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