Fumaric acid, 3-methylbutyl 2,4,6-trichlorophenyl ester

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

InchiKey: HWGBOSXEIFMYRK-ONEGZZNKSA-N

Formula: C15H15Cl3O4

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

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-266.91	kJ/mol	Joback Method
hf	-575.69	kJ/mol	Joback Method
hfus	42.32	kJ/mol	Joback Method
hvap	84.28	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.698		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	852.81	K	Joback Method
tc	1077.69	K	Joback Method
tf	536.79	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.91	J/mol×K	852.81	Joback Method
cpg	648.82	J/mol×K	890.29	Joback Method
cpg	658.78	J/mol×K	927.77	Joback Method
cpg	667.80	J/mol×K	965.25	Joback Method
cpg	675.91	J/mol×K	1002.73	Joback Method
cpg	683.13	J/mol×K	1040.21	Joback Method
cpg	689.48	J/mol×K	1077.69	Joback Method
dvisc	0.0004255	Pa×s	536.79	Joback Method

dvisc	0.0002640	Pa×s	589.46	Joback Method
dvisc	0.0001772	Pa×s	642.13	Joback Method
dvisc	0.0001263	Pa×s	694.80	Joback Method
dvisc	0.0000944	Pa×s	747.47	Joback Method
dvisc	0.0000734	Pa×s	800.14	Joback Method
dvisc	0.0000588	Pa×s	852.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405554&Units=SI
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

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