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

Inchi: InChI=1S/C13H11Cl3O4/c1-2-5-19-11(17)3-4-12(18)20-10-7-8(14)6-9(15)13(10)16/h3-4,

InchiKey: PSHHEPLAPIWQBF-ONEGZZNKSA-N

Formula: C13H11Cl3O4

SMILES: CCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 337.58

Physical Properties

Property code	Value	Unit	Source
gf	-281.31	kJ/mol	Joback Method
hf	-529.13	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.062		Crippen Method
mcvol	217.570	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	807.49	K	Joback Method
tc	1034.36	K	Joback Method
tf	529.25	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.48	J/mol×K	807.49	Joback Method
cpg	571.06	J/mol×K	996.55	Joback Method
cpg	564.38	J/mol×K	958.73	Joback Method
cpg	556.89	J/mol×K	920.92	Joback Method
cpg	548.59	J/mol×K	883.11	Joback Method
cpg	539.45	J/mol×K	845.30	Joback Method
cpg	576.95	J/mol×K	1034.36	Joback Method
dvisc	0.0000843	Pa×s	807.49	Joback Method

dvisc	0.0001029	Pa×s	761.12	Joback Method
dvisc	0.0001289	Pa×s	714.74	Joback Method
dvisc	0.0001666	Pa×s	668.37	Joback Method
dvisc	0.0002237	Pa×s	622.00	Joback Method
dvisc	0.0003149	Pa×s	575.62	Joback Method
dvisc	0.0004707	Pa×s	529.25	Joback Method

Sources

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=U348140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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