

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

Inchi:	InChI=1S/C13H11Cl3O4/c1-2-7-19-10(17)5-6-11(18)20-13-9(15)4-3-8(14)12(13)16/h3-6
InchiKey:	HXALDMWGQWGCOL-AATRIKPKSA-N
Formula:	C13H11Cl3O4
SMILES:	CCCOC(=O)C=CC(=O)Oc1c(Cl)ccc(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	2241.00		NIST Webbook
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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/molxK	807.49	Joback Method
cpg	571.06	J/molxK	996.55	Joback Method
cpg	564.38	J/molxK	958.73	Joback Method
cpg	556.89	J/molxK	920.92	Joback Method
cpg	548.59	J/molxK	883.11	Joback Method
cpg	539.45	J/molxK	845.30	Joback Method
cpg	576.95	J/molxK	1034.36	Joback Method
dvisc	0.0000843	Paxs	807.49	Joback Method

dvisc	0.0001029	Paxs	761.12	Joback Method
dvisc	0.0001289	Paxs	714.74	Joback Method
dvisc	0.0001666	Paxs	668.37	Joback Method
dvisc	0.0002237	Paxs	622.00	Joback Method
dvisc	0.0003149	Paxs	575.62	Joback Method
dvisc	0.0004707	Paxs	529.25	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=U348220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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