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

Inchi: InChI=1S/C17H19Cl3O4/c1-2-3-4-5-6-11-23-14(21)9-10-15(22)24-17-13(19)8-7-12(18)16

InchiKey: DUQKLYISVMGEDJ-MDZDMXLPSA-N

Formula: C17H19Cl3O4

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

Mol. weight [g/mol]: 393.69

Physical Properties

Property code	Value	Unit	Source
gf	-247.63	kJ/mol	Joback Method
hf	-611.69	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	89.12	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.622		Crippen Method
mcvol	273.930	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook
tb	899.01	K	Joback Method
tc	1118.59	K	Joback Method
tf	574.33	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.89	J/mol×K	899.01	Joback Method
cpg	760.30	J/mol×K	935.61	Joback Method
cpg	770.72	J/mol×K	972.20	Joback Method
cpg	780.19	J/mol×K	1008.80	Joback Method
cpg	788.72	J/mol×K	1045.40	Joback Method
cpg	796.34	J/mol×K	1082.00	Joback Method
cpg	803.09	J/mol×K	1118.59	Joback Method
dvisc	0.0003225	Pa×s	574.33	Joback Method

dvisc	0.0002051	Pa×s	628.44	Joback Method
dvisc	0.0001402	Pa×s	682.56	Joback Method
dvisc	0.0001013	Pa×s	736.67	Joback Method
dvisc	0.0000766	Pa×s	790.78	Joback Method
dvisc	0.0000600	Pa×s	844.90	Joback Method
dvisc	0.0000484	Pa×s	899.01	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=U348226&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