Fumaric acid, 2,4,6-trichlorophenyl hept-2-yl ester

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

InchiKey: QEHXDBTXKAHXSJ-BQYQJAHWSA-N

Formula: C17H19Cl3O4

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

Mol. weight [g/mol]: 393.69

Physical Properties

Property code	Value	Unit	Source
gf	-250.07	kJ/mol	Joback Method
hf	-616.97	kJ/mol	Joback Method
hfus	47.50	kJ/mol	Joback Method
hvap	88.73	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.620		Crippen Method
mcvol	273.930	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	898.57	K	Joback Method
tc	1120.45	K	Joback Method
tf	559.33	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.43	J/mol×K	898.57	Joback Method
cpg	796.97	J/mol×K	1083.47	Joback Method
cpg	789.39	J/mol×K	1046.49	Joback Method
cpg	780.88	J/mol×K	1009.51	Joback Method
cpg	771.40	J/mol×K	972.53	Joback Method
cpg	760.93	J/mol×K	935.55	Joback Method
cpg	803.64	J/mol×K	1120.45	Joback Method
dvisc	0.0000442	Pa×s	898.57	Joback Method

dvisc	0.0000555	Pa×s	842.03	Joback Method
dvisc	0.0000721	Pa×s	785.49	Joback Method
dvisc	0.0000975	Pa×s	728.95	Joback Method
dvisc	0.0001387	Pa×s	672.41	Joback Method
dvisc	0.0002104	Pa×s	615.87	Joback Method
dvisc	0.0003475	Pa×s	559.33	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=U405954&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