Fumaric acid, heptyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C17H18Cl4O4/c1-2-3-4-5-6-9-24-13(22)7-8-14(23)25-17-15(20)11(18)10-12(19

InchiKey: YUUNIIFPLKPIJX-BQYQJAHWSA-N

Formula: C17H18Cl4O4

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

Mol. weight [g/mol]: 428.13

Physical Properties

Property code	Value	Unit	Source
gf	-269.19	kJ/mol	Joback Method
hf	-638.90	kJ/mol	Joback Method
hfus	54.83	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.275		Crippen Method
mcvol	286.170	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	941.42	K	Joback Method
tc	1166.25	K	Joback Method
tf	616.77	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.66	J/mol×K	941.42	Joback Method
cpg	809.07	J/mol×K	1128.78	Joback Method
cpg	802.70	J/mol×K	1091.30	Joback Method
cpg	795.40	J/mol×K	1053.83	Joback Method
cpg	787.14	J/mol×K	1016.36	Joback Method
cpg	777.90	J/mol×K	978.89	Joback Method
cpg	814.53	J/mol×K	1166.25	Joback Method
dvisc	0.0000420	Pa×s	941.42	Joback Method

dvisc	0.0000515	Pa×s	887.31	Joback Method
dvisc	0.0000648	Pa×s	833.20	Joback Method
dvisc	0.0000842	Pa×s	779.10	Joback Method
dvisc	0.0001137	Pa×s	724.99	Joback Method
dvisc	0.0001612	Pa×s	670.88	Joback Method
dvisc	0.0002430	Pa×s	616.77	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=U348253&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