Fumaric acid, isohexyl pentachlorophenyl ester

Inchi: InChI=1S/C16H15Cl5O4/c1-8(2)4-3-7-24-9(22)5-6-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: BYHQDWGIFGHXMT-AATRIKPKSA-N

Formula: C16H15Cl5O4

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

Mol. weight [g/mol]: 448.55

Physical Properties

Property code	Value	Unit	Source
gf	-301.61	kJ/mol	Joback Method
hf	-650.75	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	96.60	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.395		Crippen Method
mcvol	284.320	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2867.00		NIST Webbook
tb	960.51	K	Joback Method
tc	1192.81	K	Joback Method
tf	632.94	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.43	J/mol×K	960.51	Joback Method
cpg	737.24	J/mol×K	999.23	Joback Method
cpg	745.03	J/mol×K	1037.94	Joback Method
cpg	751.82	J/mol×K	1076.66	Joback Method
cpg	757.63	J/mol×K	1115.38	Joback Method
cpg	762.46	J/mol×K	1154.09	Joback Method
cpg	766.34	J/mol×K	1192.81	Joback Method
dvisc	0.0002160	Pa×s	632.94	Joback Method
dvisc	0.0001446	Pa×s	687.54	Joback Method

dvisc	0.0001026	Pa×s	742.13	Joback Method
dvisc	0.0000764	Pa×s	796.73	Joback Method
dvisc	0.0000590	Pa×s	851.32	Joback Method
dvisc	0.0000471	Pa×s	905.91	Joback Method
dvisc	0.0000385	Pa×s	960.51	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=U348183&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