Fumaric acid, isohexyl 2,3,4,5-tetrachlorophenyl ester

Inchi: InChI=1S/C16H16Cl4O4/c1-9(2)4-3-7-23-12(21)5-6-13(22)24-11-8-10(17)14(18)16(20)15

InchiKey: ZIJTYAMLAPSFSL-AATRIKPKSA-N

Formula: C16H16Cl4O4

SMILES: CC(C)CCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 414.11

Physical Properties

Property code	Value	Unit	Source
gf	-280.05	kJ/mol	Joback Method
hf	-623.54	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	91.56	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.741		Crippen Method
mcvol	272.080	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	918.10	K	Joback Method
tc	1145.61	K	Joback Method
tf	590.50	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.78	J/mol×K	918.10	Joback Method
cpg	721.80	J/mol×K	956.02	Joback Method
cpg	730.82	J/mol×K	993.94	Joback Method
cpg	738.87	J/mol×K	1031.86	Joback Method
cpg	745.96	J/mol×K	1069.77	Joback Method
cpg	752.12	J/mol×K	1107.69	Joback Method
cpg	757.36	J/mol×K	1145.61	Joback Method
dvisc	0.0002859	Pa×s	590.50	Joback Method
dvisc	0.0001838	Pa×s	645.10	Joback Method

dvisc	0.0001266	Pa×s	699.70	Joback Method
dvisc	0.0000921	Pa×s	754.30	Joback Method
dvisc	0.0000699	Pa×s	808.90	Joback Method
dvisc	0.0000549	Pa×s	863.50	Joback Method
dvisc	0.0000444	Pa×s	918.10	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=U348244&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