Fumaric acid, hexyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C16H16Cl4O4/c1-2-3-4-5-8-23-12(21)6-7-13(22)24-16-11(18)9-10(17)14(19)15

InchiKey: CAUPBJYBDQEJAL-VOTSOKGWSA-N

Formula: C16H16Cl4O4

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

Mol. weight [g/mol]: 414.11

Physical Properties

Property code	Value	Unit	Source
gf	-277.61	kJ/mol	Joback Method
hf	-618.26	kJ/mol	Joback Method
hfus	52.24	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.885		Crippen Method
mcvol	272.080	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	918.54	K	Joback Method
tc	1143.65	K	Joback Method
tf	605.50	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.23	J/mol×K	918.54	Joback Method
cpg	721.19	J/mol×K	956.06	Joback Method
cpg	730.19	J/mol×K	993.58	Joback Method
cpg	738.25	J/mol×K	1031.10	Joback Method
cpg	745.38	J/mol×K	1068.61	Joback Method
cpg	751.61	J/mol×K	1106.13	Joback Method
cpg	756.96	J/mol×K	1143.65	Joback Method
dvisc	0.0002699	Pa×s	605.50	Joback Method

dvisc	0.0001811	Pa×s	657.67	Joback Method
dvisc	0.0001289	Pa×s	709.85	Joback Method
dvisc	0.0000961	Pa×s	762.02	Joback Method
dvisc	0.0000744	Pa×s	814.19	Joback Method
dvisc	0.0000594	Pa×s	866.37	Joback Method
dvisc	0.0000487	Pa×s	918.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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