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

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

InchiKey: OFPNLEPZXPVEHX-VOTSOKGWSA-N

Formula: C16H16Cl4O4

SMILES: CCCCCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)cc(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	2701.00		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	751.61	J/mol×K	1106.13	Joback Method
cpg	745.38	J/mol×K	1068.61	Joback Method
cpg	738.25	J/mol×K	1031.10	Joback Method
cpg	730.19	J/mol×K	993.58	Joback Method
cpg	721.19	J/mol×K	956.06	Joback Method
cpg	756.96	J/mol×K	1143.65	Joback Method
dvisc	0.0000487	Pa×s	918.54	Joback Method
dvisc	0.0000594	Pa×s	866.37	Joback Method

dvisc	0.0000744	Pa×s	814.19	Joback Method
dvisc	0.0000961	Pa×s	762.02	Joback Method
dvisc	0.0001289	Pa×s	709.85	Joback Method
dvisc	0.0001811	Pa×s	657.67	Joback Method
dvisc	0.0002699	Pa×s	605.50	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348252&Units=SI

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