

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

Inchi:	InChI=1S/C16H16Cl4O4/c1-2-3-4-5-8-23-12(21)6-7-13(22)24-11-9-10(17)14(18)16(20)15
InchiKey:	DRNXHSLSDLPUCA-VOTSOKGWSA-N
Formula:	C16H16Cl4O4
SMILES:	CCCCCOC(=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	-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
rinsol	2786.00		NIST Webbook
tb	918.54	K	Joback Method
tc	1143.65	K	Joback Method
tf	605.50	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.23	J/molxK	918.54	Joback Method
cpg	751.61	J/molxK	1106.13	Joback Method
cpg	745.38	J/molxK	1068.61	Joback Method
cpg	738.25	J/molxK	1031.10	Joback Method
cpg	730.19	J/molxK	993.58	Joback Method
cpg	721.19	J/molxK	956.06	Joback Method
cpg	756.96	J/molxK	1143.65	Joback Method
dvisc	0.0000487	Paxs	918.54	Joback Method
dvisc	0.0000594	Paxs	866.37	Joback Method

dvisc	0.0000744	Paxs	814.19	Joback Method
dvisc	0.0000961	Paxs	762.02	Joback Method
dvisc	0.0001289	Paxs	709.85	Joback Method
dvisc	0.0001811	Paxs	657.67	Joback Method
dvisc	0.0002699	Paxs	605.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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