

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

Inchi:	InChI=1S/C15H14Cl4O4/c1-2-3-4-7-22-11(20)5-6-12(21)23-15-13(18)9(16)8-10(17)14(19)
InchiKey:	SPGQBUMQGUSKMU-AATRIKPKSA-N
Formula:	C15H14Cl4O4
SMILES:	CCCCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	400.08

Physical Properties

Property code	Value	Unit	Source
gf	-286.03	kJ/mol	Joback Method
hf	-597.62	kJ/mol	Joback Method
hfus	49.65	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.495		Crippen Method
mcvol	257.990	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2593.00		NIST Webbook
tb	895.66	K	Joback Method
tc	1121.83	K	Joback Method
tf	594.23	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.59	J/molxK	895.66	Joback Method
cpg	665.24	J/molxK	933.36	Joback Method
cpg	673.96	J/molxK	971.05	Joback Method
cpg	681.78	J/molxK	1008.75	Joback Method
cpg	688.71	J/molxK	1046.44	Joback Method
cpg	694.76	J/molxK	1084.14	Joback Method
cpg	699.95	J/molxK	1121.83	Joback Method
dvisc	0.0002987	Paxs	594.23	Joback Method
dvisc	0.0002029	Paxs	644.47	Joback Method

dvisc	0.0001457	Paxs	694.71	Joback Method
dvisc	0.0001094	Paxs	744.95	Joback Method
dvisc	0.0000852	Paxs	795.18	Joback Method
dvisc	0.0000684	Paxs	845.42	Joback Method
dvisc	0.0000562	Paxs	895.66	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=U348250&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

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