

Fumaric acid, pentachlorophenyl pentyl ester

Inchi: InChI=1S/C15H13Cl5O4/c1-2-3-4-7-23-8(21)5-6-9(22)24-15-13(19)11(17)10(16)12(18)14
InchiKey: VLYJINNDRWZADO-AATRIKPKSA-N
Formula: C15H13Cl5O4
SMILES: CCCCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 434.53

Physical Properties

Property code	Value	Unit	Source
gf	-307.59	kJ/mol	Joback Method
hf	-624.83	kJ/mol	Joback Method
hfus	53.46	kJ/mol	Joback Method
hvap	94.77	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.149		Crippen Method
mcvol	270.230	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2804.00		NIST Webbook
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tb	938.07	K	Joback Method
tc	1168.76	K	Joback Method
tf	636.67	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.05	J/molxK	938.07	Joback Method
cpg	680.55	J/molxK	976.52	Joback Method
cpg	688.11	J/molxK	1014.97	Joback Method
cpg	694.73	J/molxK	1053.41	Joback Method
cpg	700.45	J/molxK	1091.86	Joback Method
cpg	705.25	J/molxK	1130.31	Joback Method
cpg	709.17	J/molxK	1168.76	Joback Method
dvisc	0.0002304	Paxs	636.67	Joback Method

dvisc	0.0001619	Paxs	686.90	Joback Method
dvisc	0.0001194	Paxs	737.14	Joback Method
dvisc	0.0000916	Paxs	787.37	Joback Method
dvisc	0.0000725	Paxs	837.60	Joback Method
dvisc	0.0000589	Paxs	887.84	Joback Method
dvisc	0.0000489	Paxs	938.07	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348182&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

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