

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

Inchi:	InChI=1S/C17H18Cl4O4/c1-2-3-4-5-6-9-24-13(22)7-8-14(23)25-17-12(19)10-11(18)15(20)
InchiKey:	GOGVZHKCOHWPGO-BQYQJAHWSA-N
Formula:	C17H18Cl4O4
SMILES:	CCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	428.13

Physical Properties

Property code	Value	Unit	Source
gf	-269.19	kJ/mol	Joback Method
hf	-638.90	kJ/mol	Joback Method
hfus	54.83	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.275		Crippen Method
mvol	286.170	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2817.00		NIST Webbook
tb	941.42	K	Joback Method
tc	1166.25	K	Joback Method
tf	616.77	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.66	J/molxK	941.42	Joback Method
cpg	777.90	J/molxK	978.89	Joback Method
cpg	787.14	J/molxK	1016.36	Joback Method
cpg	795.40	J/molxK	1053.83	Joback Method
cpg	802.70	J/molxK	1091.30	Joback Method
cpg	809.07	J/molxK	1128.78	Joback Method
cpg	814.53	J/molxK	1166.25	Joback Method
dvisc	0.0002430	Paxs	616.77	Joback Method
dvisc	0.0001612	Paxs	670.88	Joback Method

dvisc	0.0001137	Paxs	724.99	Joback Method
dvisc	0.0000842	Paxs	779.10	Joback Method
dvisc	0.0000648	Paxs	833.20	Joback Method
dvisc	0.0000515	Paxs	887.31	Joback Method
dvisc	0.0000420	Paxs	941.42	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=U348199&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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