

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

Inchi:	InChI=1S/C14H12Cl4O4/c1-7(2)6-21-10(19)3-4-11(20)22-14-9(16)5-8(15)12(17)13(14)18
InchiKey:	URUVAKSJVJOFGY-ONEGZZNKSA-N
Formula:	C14H12Cl4O4
SMILES:	CC(C)COC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	386.06

Physical Properties

Property code	Value	Unit	Source
gf	-296.89	kJ/mol	Joback Method
hf	-582.26	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	87.10	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.961		Crippen Method
mcvol	243.900	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinqol	2446.00		NIST Webbook
tb	872.34	K	Joback Method
tc	1103.40	K	Joback Method
tf	567.96	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.41	J/molxK	872.34	Joback Method
cpg	639.23	J/molxK	1064.89	Joback Method
cpg	633.45	J/molxK	1026.38	Joback Method
cpg	626.80	J/molxK	987.87	Joback Method
cpg	619.25	J/molxK	949.36	Joback Method
cpg	610.79	J/molxK	910.85	Joback Method
cpg	644.13	J/molxK	1103.40	Joback Method
dvisc	0.0000593	Paxs	872.34	Joback Method
dvisc	0.0000727	Paxs	821.61	Joback Method

dvisc	0.0000917	Paxs	770.88	Joback Method
dvisc	0.0001194	Paxs	720.15	Joback Method
dvisc	0.0001619	Paxs	669.42	Joback Method
dvisc	0.0002308	Paxs	618.69	Joback Method
dvisc	0.0003504	Paxs	567.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348194&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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