

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

Inchi:	InChI=1S/C14H12Cl4O4/c1-2-3-6-21-10(19)4-5-11(20)22-14-9(16)7-8(15)12(17)13(14)18
InchiKey:	BPFAPIRCWGTJKJ-SNAWJCMRSA-N
Formula:	C14H12Cl4O4
SMILES:	CCCCOC(=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	-294.45	kJ/mol	Joback Method
hf	-576.98	kJ/mol	Joback Method
hfus	47.06	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.105		Crippen Method
mcvol	243.900	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	872.78	K	Joback Method
tc	1100.74	K	Joback Method
tf	582.96	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.80	J/molxK	872.78	Joback Method
cpg	610.09	J/molxK	910.77	Joback Method
cpg	618.50	J/molxK	948.77	Joback Method
cpg	626.03	J/molxK	986.76	Joback Method
cpg	632.71	J/molxK	1024.75	Joback Method
cpg	638.54	J/molxK	1062.74	Joback Method
cpg	643.53	J/molxK	1100.74	Joback Method
dvisc	0.0003294	Paxs	582.96	Joback Method

dvisc	0.0002264	Paxs	631.26	Joback Method
dvisc	0.0001642	Paxs	679.57	Joback Method
dvisc	0.0001242	Paxs	727.87	Joback Method
dvisc	0.0000973	Paxs	776.17	Joback Method
dvisc	0.0000785	Paxs	824.48	Joback Method
dvisc	0.0000648	Paxs	872.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348195&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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