

Fumaric acid, butyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C14H13Cl3O4/c1-2-3-6-20-12(18)4-5-13(19)21-9-7-10(15)14(17)11(16)8-9/h4-
InchiKey:	DMECDNPDAOOMEY-SNAWJCMRSA-N
Formula:	C14H13Cl3O4
SMILES:	CCCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	351.61

Physical Properties

Property code	Value	Unit	Source
gf	-272.89	kJ/mol	Joback Method
hf	-549.77	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	82.44	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.452		Crippen Method
mvol	231.660	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2408.00		NIST Webbook
tb	830.37	K	Joback Method
tc	1054.44	K	Joback Method
tf	540.52	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.90	J/molxK	830.37	Joback Method
cpg	593.31	J/molxK	867.72	Joback Method
cpg	602.84	J/molxK	905.06	Joback Method
cpg	611.51	J/molxK	942.41	Joback Method
cpg	619.33	J/molxK	979.75	Joback Method
cpg	626.32	J/molxK	1017.10	Joback Method
cpg	632.50	J/molxK	1054.44	Joback Method
dvisc	0.0004310	Paxs	540.52	Joback Method
dvisc	0.0002846	Paxs	588.83	Joback Method

dvisc	0.0002001	Paxs	637.14	Joback Method
dvisc	0.0001479	Paxs	685.45	Joback Method
dvisc	0.0001137	Paxs	733.75	Joback Method
dvisc	0.0000903	Paxs	782.06	Joback Method
dvisc	0.0000737	Paxs	830.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348152&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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