

Fumaric acid, isobutyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C14H13Cl3O4/c1-8(2)7-20-12(18)3-4-13(19)21-14-10(16)5-9(15)6-11(14)17/h3
InchiKey:	JJOFXKGOYZAVLR-ONEGZZNKSA-N
Formula:	C14H13Cl3O4
SMILES:	CC(C)COC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	351.61

Physical Properties

Property code	Value	Unit	Source
gf	-275.33	kJ/mol	Joback Method
hf	-555.05	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.308		Crippen Method
mcvol	231.660	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2216.00		NIST Webbook
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tb	829.93	K	Joback Method
tc	1057.31	K	Joback Method
tf	525.52	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.51	J/molxK	829.93	Joback Method
cpg	594.06	J/molxK	867.83	Joback Method
cpg	603.69	J/molxK	905.72	Joback Method
cpg	612.41	J/molxK	943.62	Joback Method
cpg	620.25	J/molxK	981.52	Joback Method
cpg	627.23	J/molxK	1019.41	Joback Method
cpg	633.35	J/molxK	1057.31	Joback Method
dvisc	0.0004680	Paxs	525.52	Joback Method

dvisc	0.0002941	Paxs	576.25	Joback Method
dvisc	0.0001993	Paxs	626.99	Joback Method
dvisc	0.0001431	Paxs	677.72	Joback Method
dvisc	0.0001076	Paxs	728.46	Joback Method
dvisc	0.0000840	Paxs	779.19	Joback Method
dvisc	0.0000676	Paxs	829.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348269&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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