

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

Inchi:	InChI=1S/C19H23Cl3O4/c1-2-3-4-5-6-7-8-11-25-17(23)9-10-18(24)26-19-15(21)12-14(20)
InchiKey:	IKTKSBWABKVBNL-MDZDMXLPSA-N
Formula:	C19H23Cl3O4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	421.74

Physical Properties

Property code	Value	Unit	Source
gf	-230.79	kJ/mol	Joback Method
hf	-652.97	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	93.57	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.402		Crippen Method
mvol	302.110	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	944.77	K	Joback Method
tc	1165.05	K	Joback Method
tf	596.87	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.64	J/molxK	944.77	Joback Method
cpg	875.57	J/molxK	981.48	Joback Method
cpg	886.43	J/molxK	1018.20	Joback Method
cpg	896.26	J/molxK	1054.91	Joback Method
cpg	905.10	J/molxK	1091.63	Joback Method
cpg	912.97	J/molxK	1128.34	Joback Method
cpg	919.92	J/molxK	1165.05	Joback Method
dvisc	0.0002609	Paxs	596.87	Joback Method

dvisc	0.0001621	Paxs	654.85	Joback Method
dvisc	0.0001089	Paxs	712.84	Joback Method
dvisc	0.0000776	Paxs	770.82	Joback Method
dvisc	0.0000580	Paxs	828.80	Joback Method
dvisc	0.0000451	Paxs	886.79	Joback Method
dvisc	0.0000361	Paxs	944.77	Joback Method

Sources

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=U348276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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