

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

Inchi:	InChI=1S/C18H21Cl3O4/c1-3-5-6-12(4-2)11-24-16(22)7-8-17(23)25-18-14(20)9-13(19)10
InchiKey:	QJGOSRJMONNBOU-BQYQJAHWSA-N
Formula:	C18H21Cl3O4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	407.72

Physical Properties

Property code	Value	Unit	Source
gf	-241.65	kJ/mol	Joback Method
hf	-637.61	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.868		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinsol	2597.00		NIST Webbook
rinsol	2597.00		NIST Webbook
tb	921.45	K	Joback Method
tc	1142.93	K	Joback Method
tf	570.60	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.41	J/molxK	921.45	Joback Method
cpg	818.15	J/molxK	958.36	Joback Method
cpg	828.83	J/molxK	995.28	Joback Method
cpg	838.49	J/molxK	1032.19	Joback Method
cpg	847.16	J/molxK	1069.10	Joback Method
cpg	854.86	J/molxK	1106.02	Joback Method
cpg	861.63	J/molxK	1142.93	Joback Method
dvisc	0.0003122	Paxs	570.60	Joback Method

dvisc	0.0001869	Paxs	629.08	Joback Method
dvisc	0.0001221	Paxs	687.55	Joback Method
dvisc	0.0000853	Paxs	746.02	Joback Method
dvisc	0.0000627	Paxs	804.50	Joback Method
dvisc	0.0000481	Paxs	862.97	Joback Method
dvisc	0.0000382	Paxs	921.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405956&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

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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