

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-239.21	kJ/mol	Joback Method
hf	-632.33	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.012		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	921.89	K	Joback Method
tc	1141.42	K	Joback Method
tf	585.60	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.90	J/molxK	921.89	Joback Method
cpg	817.57	J/molxK	958.48	Joback Method
cpg	828.23	J/molxK	995.07	Joback Method
cpg	837.89	J/molxK	1031.66	Joback Method
cpg	846.58	J/molxK	1068.25	Joback Method
cpg	854.35	J/molxK	1104.83	Joback Method
cpg	861.21	J/molxK	1141.42	Joback Method
dvisc	0.0002906	Paxs	585.60	Joback Method
dvisc	0.0001827	Paxs	641.65	Joback Method

dvisc	0.0001237	Paxs	697.70	Joback Method
dvisc	0.0000888	Paxs	753.75	Joback Method
dvisc	0.0000667	Paxs	809.79	Joback Method
dvisc	0.0000520	Paxs	865.84	Joback Method
dvisc	0.0000418	Paxs	921.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348275&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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