

Fumaric acid, decyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C20H25Cl3O4/c1-2-3-4-5-6-7-8-9-14-26-17(24)12-13-18(25)27-20-16(22)11-10
InchiKey:	UKPVUYCTLVSBPN-OUKQBFOZSA-N
Formula:	C20H25Cl3O4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	435.77

Physical Properties

Property code	Value	Unit	Source
gf	-222.37	kJ/mol	Joback Method
hf	-673.61	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.792		Crippen Method
mcvol	316.200	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinqol	3004.00		NIST Webbook
tb	967.65	K	Joback Method
tc	1189.54	K	Joback Method
tf	608.14	K	Joback Method
vc	1.222	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.06	J/molxK	967.65	Joback Method
cpg	934.23	J/molxK	1004.63	Joback Method
cpg	945.29	J/molxK	1041.61	Joback Method
cpg	955.28	J/molxK	1078.60	Joback Method
cpg	964.23	J/molxK	1115.58	Joback Method
cpg	972.20	J/molxK	1152.56	Joback Method
cpg	979.20	J/molxK	1189.54	Joback Method
dvisc	0.0002335	Paxs	608.14	Joback Method
dvisc	0.0001435	Paxs	668.06	Joback Method

dvisc	0.0000956	Paxs	727.98	Joback Method
dvisc	0.0000677	Paxs	787.89	Joback Method
dvisc	0.0000504	Paxs	847.81	Joback Method
dvisc	0.0000389	Paxs	907.73	Joback Method
dvisc	0.0000311	Paxs	967.65	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=U348229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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