

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

Inchi:	InChI=1S/C23H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-29-21(27)13-14-22(28)30-23-19
InchiKey:	RFHVSCGCTYDDEL-BUHFOSPRSA-N
Formula:	C23H31Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	477.85

Physical Properties

Property code	Value	Unit	Source
gf	-197.11	kJ/mol	Joback Method
hf	-735.53	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	102.48	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	7.963		Crippen Method
mvol	358.470	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3231.00		NIST Webbook
rinpol	3231.00		NIST Webbook
tb	1036.29	K	Joback Method
tc	1268.71	K	Joback Method
tf	641.95	K	Joback Method
vc	1.391	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.85	J/molxK	1036.29	Joback Method
cpg	1113.76	J/molxK	1075.03	Joback Method
cpg	1125.39	J/molxK	1113.76	Joback Method
cpg	1135.80	J/molxK	1152.50	Joback Method
cpg	1145.03	J/molxK	1191.24	Joback Method
cpg	1153.15	J/molxK	1229.97	Joback Method
cpg	1160.22	J/molxK	1268.71	Joback Method
dvisc	0.0001644	Paxs	641.95	Joback Method

dvisc	0.0000979	Paxs	707.67	Joback Method
dvisc	0.0000637	Paxs	773.40	Joback Method
dvisc	0.0000443	Paxs	839.12	Joback Method
dvisc	0.0000325	Paxs	904.84	Joback Method
dvisc	0.0000249	Paxs	970.57	Joback Method
dvisc	0.0000197	Paxs	1036.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348277&Units=SI

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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