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

Inchi: InChI=1S/C17H10Cl4O4/c18-11-3-1-10(2-4-11)9-24-15(22)5-6-16(23)25-17-13(20)7-12(1

InchiKey: DFLILAMCVZWJHV-AATRIKPKSA-N

Formula: C17H10Cl4O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 420.07

Physical Properties

Property code	Value	Unit	Source
gf	-156.78	kJ/mol	Joback Method
hf	-402.37	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.505		Crippen Method
mcvol	262.410	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	968.10	K	Joback Method
tc	1219.35	K	Joback Method
tf	643.19	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.64	J/mol×K	968.10	Joback Method
cpg	666.47	J/mol×K	1009.98	Joback Method
cpg	673.22	J/mol×K	1051.85	Joback Method
cpg	678.96	J/mol×K	1093.73	Joback Method
cpg	683.71	J/mol×K	1135.60	Joback Method
cpg	687.54	J/mol×K	1177.48	Joback Method
cpg	690.47	J/mol×K	1219.35	Joback Method
dvisc	0.0002289	Pa×s	643.19	Joback Method

dvisc	0.0001561	Pa×s	697.34	Joback Method
dvisc	0.0001125	Pa×s	751.49	Joback Method
dvisc	0.0000847	Pa×s	805.64	Joback Method
dvisc	0.0000661	Pa×s	859.80	Joback Method
dvisc	0.0000531	Pa×s	913.95	Joback Method
dvisc	0.0000437	Pa×s	968.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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