Fumaric acid, 4-chlorobenzyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H12Cl2O4/c18-13-6-4-12(5-7-13)11-22-16(20)8-9-17(21)23-15-3-1-2-14(19

InchiKey: KZGJOLRIXGDDHS-CMDGGOBGSA-N

Formula: C17H12Cl2O4

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 351.18

Physical Properties

Property code	Value	Unit	Source
gf	-113.66	kJ/mol	Joback Method
hf	-347.95	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.198		Crippen Method
mcvol	237.930	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	883.28	K	Joback Method
tc	1128.36	K	Joback Method
tf	558.31	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.22	J/mol×K	883.28	Joback Method
cpg	668.99	J/mol×K	1087.51	Joback Method
cpg	662.65	J/mol×K	1046.66	Joback Method
cpg	655.36	J/mol×K	1005.82	Joback Method
cpg	647.06	J/mol×K	964.97	Joback Method
cpg	637.70	J/mol×K	924.13	Joback Method
cpg	674.43	J/mol×K	1128.36	Joback Method
dvisc	0.0000569	Pa×s	883.28	Joback Method

dvisc	0.0000707	Pa×s	829.12	Joback Method
dvisc	0.0000905	Pa×s	774.96	Joback Method
dvisc	0.0001203	Pa×s	720.80	Joback Method
dvisc	0.0001674	Pa×s	666.63	Joback Method
dvisc	0.0002470	Pa×s	612.47	Joback Method
dvisc	0.0003929	Pa×s	558.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405922&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