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

Inchi: InChI=1S/C16H17Cl3O4/c1-10(2)4-3-7-22-14(20)5-6-15(21)23-16-12(18)8-11(17)9-13(16

InchiKey: VJWIRWKRNBZDAC-AATRIKPKSA-N

Formula: C16H17Cl3O4

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

Mol. weight [g/mol]: 379.66

Physical Properties

Property code	Value	Unit	Source
gf	-258.49	kJ/mol	Joback Method
hf	-596.33	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	86.51	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.088		Crippen Method
mcvol	259.840	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		NIST Webbook
tb	875.69	K	Joback Method
tc	1098.72	K	Joback Method
tf	548.06	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.24	J/mol×K	875.69	Joback Method
cpg	739.72	J/mol×K	1061.55	Joback Method
cpg	732.30	J/mol×K	1024.38	Joback Method
cpg	723.97	J/mol×K	987.20	Joback Method
cpg	714.70	J/mol×K	950.03	Joback Method
cpg	704.46	J/mol×K	912.86	Joback Method
cpg	746.25	J/mol×K	1098.72	Joback Method
dvisc	0.0000510	Pa×s	875.69	Joback Method

dvisc	0.0000639	Pa×s	821.09	Joback Method
dvisc	0.0000826	Pa×s	766.48	Joback Method
dvisc	0.0001111	Pa×s	711.88	Joback Method
dvisc	0.0001570	Pa×s	657.27	Joback Method
dvisc	0.0002361	Pa×s	602.67	Joback Method
dvisc	0.0003853	Pa×s	548.06	Joback Method

Sources

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=U348272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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