Fumaric acid, 3,5-dichlorophenyl hexyl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-2-3-4-5-8-21-15(19)6-7-16(20)22-14-10-12(17)9-13(18)11-14
InchiKey: HKPGBKSEDUOXAX-VOTSOKGWSA-N
Formula: C16H18Cl2O4
SMILES: CCCCCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-234.49	kJ/mol	Joback Method
hf	-563.84	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.578		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	833.72	K	Joback Method
tc	1049.62	K	Joback Method
tf	520.62	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.16	J/mol×K	833.72	Joback Method
cpg	684.45	J/mol×K	869.70	Joback Method
cpg	695.79	J/mol×K	905.69	Joback Method
cpg	706.20	J/mol×K	941.67	Joback Method
cpg	715.71	J/mol×K	977.65	Joback Method
cpg	724.35	J/mol×K	1013.64	Joback Method
cpg	732.14	J/mol×K	1049.62	Joback Method
dvisc	0.0004803	Pa×s	520.62	Joback Method

dvisc	0.0002941	Pa×s	572.80	Joback Method
dvisc	0.0001954	Pa×s	624.99	Joback Method
dvisc	0.0001383	Pa×s	677.17	Joback Method
dvisc	0.0001029	Pa×s	729.35	Joback Method
dvisc	0.0000796	Pa×s	781.54	Joback Method
dvisc	0.0000636	Pa×s	833.72	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=U348237&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