Dodecyl 2,4,6-trichlorophenyl ether

Inchi: InChI=1S/C18H27Cl3O/c1-2-3-4-5-6-7-8-9-10-11-12-22-18-16(20)13-15(19)14-17(18)21/
InchiKey: WDCCFVMECZLGEP-UHFFFAOYSA-N
Formula: C18H27Cl3O
SMILES: CCCCCCCCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 365.76

Physical Properties

Property code	Value	Unit	Source
gf	43.41	kJ/mol	Joback Method
hf	-392.17	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.946		Crippen Method
mcvol	283.310	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	787.57	K	Joback Method
tc	987.43	K	Joback Method
tf	468.59	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.25	J/mol×K	787.57	Joback Method
cpg	794.07	J/mol×K	820.88	Joback Method
cpg	808.94	J/mol×K	854.19	Joback Method
cpg	822.90	J/mol×K	887.50	Joback Method
cpg	835.96	J/mol×K	920.81	Joback Method
cpg	848.17	J/mol×K	954.12	Joback Method
cpg	859.55	J/mol×K	987.43	Joback Method
dvisc	0.0006040	Pa×s	468.59	Joback Method

dvisc	0.0003491	Pa×s	521.75	Joback Method
dvisc	0.0002233	Pa×s	574.92	Joback Method
dvisc	0.0001541	Pa×s	628.08	Joback Method
dvisc	0.0001126	Pa×s	681.24	Joback Method
dvisc	0.0000862	Pa×s	734.41	Joback Method
dvisc	0.0000683	Pa×s	787.57	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=R260194&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