Hexadecyl 2,4,6-trichlorophenyl ether

Inchi: InChI=1S/C22H35Cl3O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-26-22-20(24)17-19(23)
InchiKey: JKCZIZUDOOVIBU-UHFFFAOYSA-N
Formula: C22H35Cl3O
SMILES: CCCCCCCCCCCCCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 421.87

Physical Properties

Property code	Value	Unit	Source
gf	77.09	kJ/mol	Joback Method
hf	-474.73	kJ/mol	Joback Method
hfus	59.39	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-9.93		Crippen Method
logp	9.507		Crippen Method
mcvol	339.670	ml/mol	McGowan Method
pc	993.88	kPa	Joback Method
rinpol	2895.00		NIST Webbook
tb	879.09	K	Joback Method
tc	1081.51	K	Joback Method
tf	513.67	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.05	J/mol×K	879.09	Joback Method
cpg	1088.51	J/mol×K	1047.77	Joback Method
cpg	1075.63	J/mol×K	1014.04	Joback Method
cpg	1061.79	J/mol×K	980.30	Joback Method
cpg	1046.94	J/mol×K	946.56	Joback Method
cpg	1031.04	J/mol×K	912.83	Joback Method
cpg	1100.46	J/mol×K	1081.51	Joback Method
dvisc	0.0000391	Pa×s	879.09	Joback Method
dvisc	0.0000500	Pa×s	818.19	Joback Method

dvisc	0.0000665	Pa×s	757.28	Joback Method
dvisc	0.0000929	Pa×s	696.38	Joback Method
dvisc	0.0001384	Pa×s	635.48	Joback Method
dvisc	0.0002244	Pa×s	574.57	Joback Method
dvisc	0.0004080	Pa×s	513.67	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=R260203&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