Hexyl 2,4,6-trichlorophenyl ether

Inchi: InChI=1S/C12H15Cl3O/c1-2-3-4-5-6-16-12-10(14)7-9(13)8-11(12)15/h7-8H,2-6H2,1H3
InchiKey: WHLGHIKWAAWGGF-UHFFFAOYSA-N
Formula: C12H15Cl3O
SMILES: CCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 281.61

Physical Properties

Property code	Value	Unit	Source
gf	-7.11	kJ/mol	Joback Method
hf	-268.33	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.606		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	650.29	K	Joback Method
tc	863.25	K	Joback Method
tf	400.97	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.68	J/mol×K	650.29	Joback Method
cpg	468.81	J/mol×K	685.78	Joback Method
cpg	481.19	J/mol×K	721.28	Joback Method
cpg	492.84	J/mol×K	756.77	Joback Method
cpg	503.77	J/mol×K	792.26	Joback Method
cpg	513.99	J/mol×K	827.76	Joback Method
cpg	523.53	J/mol×K	863.25	Joback Method
dvisc	0.0009292	Pa×s	400.97	Joback Method

dvisc	0.0005877	Pa×s	442.52	Joback Method
dvisc	0.0004021	Pa×s	484.08	Joback Method
dvisc	0.0002922	Pa×s	525.63	Joback Method
dvisc	0.0002225	Pa×s	567.18	Joback Method
dvisc	0.0001758	Pa×s	608.74	Joback Method
dvisc	0.0001432	Pa×s	650.29	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=R260218&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