Tetradecyl 2,4,6-trichlorophenyl ether

Inchi: InChI=1S/C20H31Cl3O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-24-20-18(22)15-17(21)16-19(
InchiKey: SBDHUWWHEQOPBO-UHFFFAOYSA-N
Formula: C20H31Cl3O
SMILES: CCCCCCCCCCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 393.82

Physical Properties

Property code	Value	Unit	Source
gf	60.25	kJ/mol	Joback Method
hf	-433.45	kJ/mol	Joback Method
hfus	54.21	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	8.727		Crippen Method
mcvol	311.490	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2682.00		NIST Webbook
rinpol	2682.00		NIST Webbook
tb	833.33	K	Joback Method
tc	1033.08	K	Joback Method
tf	491.13	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.47	J/mol×K	833.33	Joback Method
cpg	910.87	J/mol×K	866.62	Joback Method
cpg	926.27	J/mol×K	899.91	Joback Method
cpg	940.69	J/mol×K	933.21	Joback Method
cpg	954.17	J/mol×K	966.50	Joback Method
cpg	966.74	J/mol×K	999.79	Joback Method
cpg	978.43	J/mol×K	1033.08	Joback Method
dvisc	0.0005007	Pa×s	491.13	Joback Method

dvisc	0.0002820	Pa×s	548.16	Joback Method
dvisc	0.0001770	Pa×s	605.20	Joback Method
dvisc	0.0001204	Pa×s	662.23	Joback Method
dvisc	0.0000870	Pa×s	719.26	Joback Method
dvisc	0.0000660	Pa×s	776.30	Joback Method
dvisc	0.0000520	Pa×s	833.33	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=R260238&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