

1,2,4-Trichloro-5-[(2-ethylhexyl)oxy]benzene

Inchi:	InChI=1S/C14H19Cl3O/c1-3-5-6-10(4-2)9-18-14-8-12(16)11(15)7-13(14)17/h7-8,10H,3-6
InchiKey:	RARCMPNWEIHMRC-UHFFFAOYSA-N
Formula:	C14H19Cl3O
SMILES:	CCCCC(CC)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	309.66
CAS:	107559-24-0

Physical Properties

Property code	Value	Unit	Source
gf	7.29	kJ/mol	Joback Method
hf	-314.89	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.242		Crippen Method
mvol	226.950	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	695.61	K	Joback Method
tc	906.04	K	Joback Method
tf	408.51	K	Joback Method
vc	0.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.75	J/molxK	695.61	Joback Method
cpg	573.30	J/molxK	730.68	Joback Method
cpg	586.99	J/molxK	765.75	Joback Method
cpg	599.84	J/molxK	800.83	Joback Method
cpg	611.86	J/molxK	835.90	Joback Method
cpg	623.09	J/molxK	870.97	Joback Method
cpg	633.53	J/molxK	906.04	Joback Method
dvisc	0.0009542	Paxs	408.51	Joback Method
dvisc	0.0005450	Paxs	456.36	Joback Method

dvisc	0.0003462	Paxs	504.21	Joback Method
dvisc	0.0002379	Paxs	552.06	Joback Method
dvisc	0.0001736	Paxs	599.91	Joback Method
dvisc	0.0001327	Paxs	647.76	Joback Method
dvisc	0.0001052	Paxs	695.61	Joback Method

Sources

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=C107559240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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