

Octyl 2,4,6-trichlorophenyl ether

Inchi:	InChI=1S/C14H19Cl3O/c1-2-3-4-5-6-7-8-18-14-12(16)9-11(15)10-13(14)17/h9-10H,2-8H
InchiKey:	DZXMKDOJKVKXDB-UHFFFAOYSA-N
Formula:	C14H19Cl3O
SMILES:	CCCCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	309.66

Physical Properties

Property code	Value	Unit	Source
gf	9.73	kJ/mol	Joback Method
hf	-309.61	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.386		Crippen Method
mvol	226.950	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
tb	696.05	K	Joback Method
tc	902.88	K	Joback Method
tf	423.51	K	Joback Method
vc	0.876	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.21	J/molxK	696.05	Joback Method
cpg	621.57	J/molxK	868.41	Joback Method
cpg	610.47	J/molxK	833.93	Joback Method
cpg	598.60	J/molxK	799.46	Joback Method
cpg	585.95	J/molxK	764.99	Joback Method
cpg	572.49	J/molxK	730.52	Joback Method
cpg	631.93	J/molxK	902.88	Joback Method
dvisc	0.0001137	Paxs	696.05	Joback Method

dvisc	0.0001410	Paxs	650.63	Joback Method
dvisc	0.0001806	Paxs	605.20	Joback Method
dvisc	0.0002407	Paxs	559.78	Joback Method
dvisc	0.0003377	Paxs	514.36	Joback Method
dvisc	0.0005057	Paxs	468.93	Joback Method
dvisc	0.0008258	Paxs	423.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R260223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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