

Decyl 2,4,6-trichlorophenyl ether

Inchi:	InChI=1S/C16H23Cl3O/c1-2-3-4-5-6-7-8-9-10-20-16-14(18)11-13(17)12-15(16)19/h11-12
InchiKey:	DHMMWYWZWRXZRK-UHFFFAOYSA-N
Formula:	C16H23Cl3O
SMILES:	CCCCCCCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	337.71

Physical Properties

Property code	Value	Unit	Source
gf	26.57	kJ/mol	Joback Method
hf	-350.89	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	7.166		Crippen Method
mvol	255.130	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	741.81	K	Joback Method
tc	944.15	K	Joback Method
tf	446.05	K	Joback Method
vc	0.989	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.96	J/molxK	741.81	Joback Method
cpg	681.10	J/molxK	775.53	Joback Method
cpg	695.35	J/molxK	809.26	Joback Method
cpg	708.75	J/molxK	842.98	Joback Method
cpg	721.30	J/molxK	876.70	Joback Method
cpg	733.04	J/molxK	910.43	Joback Method
cpg	743.99	J/molxK	944.15	Joback Method
dvisc	0.0007144	Paxs	446.05	Joback Method

dvisc	0.0004245	Paxs	495.34	Joback Method
dvisc	0.0002772	Paxs	544.64	Joback Method
dvisc	0.0001943	Paxs	593.93	Joback Method
dvisc	0.0001438	Paxs	643.22	Joback Method
dvisc	0.0001111	Paxs	692.52	Joback Method
dvisc	0.0000888	Paxs	741.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R260189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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