

Alpha,alpha,alpha,alpha',alpha'-pentachloro-o-xyl

Other names:	1-(dichloromethyl)-2-(trichloromethyl)benzene
Inchi:	InChI=1S/C8H5Cl5/c9-7(10)5-3-1-2-4-6(5)8(11,12)13/h1-4,7H
InchiKey:	UXMNSLMVCBBGCW-UHFFFAOYSA-N
Formula:	C8H5Cl5
SMILES:	<chem>C1C(Cl)c1cccc1C(Cl)(Cl)Cl</chem>
Mol. weight [g/mol]:	278.39
CAS:	2741-57-3

Physical Properties

Property code	Value	Unit	Source
gf	60.01	kJ/mol	Joback Method
hf	-76.12	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.989		Crippen Method
mcvol	161.020	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	597.58	K	Joback Method
tc	856.82	K	Joback Method
tf	355.88	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.92	J/molxK	597.58	Joback Method
cpg	334.24	J/molxK	813.62	Joback Method
cpg	328.38	J/molxK	770.41	Joback Method
cpg	321.81	J/molxK	727.20	Joback Method
cpg	314.44	J/molxK	683.99	Joback Method
cpg	306.18	J/molxK	640.79	Joback Method
cpg	339.50	J/molxK	856.82	Joback Method
dvisc	0.0002069	Paxs	597.58	Joback Method

dvisc	0.0002693	Paxs	557.30	Joback Method
dvisc	0.0003653	Paxs	517.01	Joback Method
dvisc	0.0005217	Paxs	476.73	Joback Method
dvisc	0.0007958	Paxs	436.45	Joback Method
dvisc	0.0013227	Paxs	396.16	Joback Method
dvisc	0.0024665	Paxs	355.88	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=C2741573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/26-782-5/Alpha-alpha-alpha-alpha-alpha-pentachloro-o-xylene.pdf>

Generated by Cheméo on 2024-04-25 17:19:08.605767161 +0000 UTC m=+16354797.526344473.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.