

2,3,6-Trichloro-4-propylphenol

Inchi:	InChI=1S/C9H9Cl3O/c1-2-3-5-4-6(10)9(13)8(12)7(5)11/h4,13H,2-3H2,1H3
InchiKey:	GJOZUMXBGLUAJG-UHFFFAOYSA-N
Formula:	C9H9Cl3O
SMILES:	CCc1cc(Cl)c(O)c(Cl)c1Cl
Mol. weight [g/mol]:	239.53
CAS:	116632-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-81.99	kJ/mol	Joback Method
hf	-251.50	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.305		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	639.85	K	Joback Method
tc	877.05	K	Joback Method
tf	456.65	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.27	J/molxK	639.85	Joback Method
cpg	342.65	J/molxK	679.38	Joback Method
cpg	351.42	J/molxK	718.92	Joback Method
cpg	359.67	J/molxK	758.45	Joback Method
cpg	367.48	J/molxK	797.99	Joback Method
cpg	374.92	J/molxK	837.52	Joback Method
cpg	382.06	J/molxK	877.05	Joback Method
dvisc	0.0003944	Paxs	456.65	Joback Method
dvisc	0.0002258	Paxs	487.18	Joback Method

dvisc	0.0001380	Paxs	517.72	Joback Method
dvisc	0.0000892	Paxs	548.25	Joback Method
dvisc	0.0000603	Paxs	578.78	Joback Method
dvisc	0.0000424	Paxs	609.32	Joback Method
dvisc	0.0000308	Paxs	639.85	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=C116632996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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/49-865-8/2-3-6-Trichloro-4-propylphenol.pdf>

Generated by Cheméo on 2024-04-29 10:12:54.525227733 +0000 UTC m=+16674823.445805045.

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