

3,6-Dichloro-2-propyl phenol

Inchi:	InChI=1S/C9H10Cl2O/c1-2-3-6-7(10)4-5-8(11)9(6)12/h4-5,12H,2-3H2,1H3
InchiKey:	ITRKBGGUVDEKOC-UHFFFAOYSA-N
Formula:	C9H10Cl2O
SMILES:	CCc1c(Cl)ccc(Cl)c1O
Mol. weight [g/mol]:	205.08
CAS:	116632-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-60.43	kJ/mol	Joback Method
hf	-224.29	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	61.01	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.651		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	597.44	K	Joback Method
tc	830.40	K	Joback Method
tf	414.21	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.50	J/molxK	597.44	Joback Method
cpg	323.94	J/molxK	636.27	Joback Method
cpg	333.68	J/molxK	675.09	Joback Method
cpg	342.79	J/molxK	713.92	Joback Method
cpg	351.35	J/molxK	752.75	Joback Method
cpg	359.43	J/molxK	791.57	Joback Method
cpg	367.12	J/molxK	830.40	Joback Method
dvisc	0.0007683	Paxs	414.21	Joback Method
dvisc	0.0003995	Paxs	444.75	Joback Method

dvisc	0.0002260	Paxs	475.29	Joback Method
dvisc	0.0001369	Paxs	505.83	Joback Method
dvisc	0.0000878	Paxs	536.36	Joback Method
dvisc	0.0000591	Paxs	566.90	Joback Method
dvisc	0.0000414	Paxs	597.44	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=C116632963&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
mcvol:	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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