2,4,6-Trichlorophenol, n-butyl ether

Other names: Butyl 2,4,6-trichlorophenyl ether
Inchi: InChI=1S/C10H11Cl3O/c1-2-3-4-14-10-8(12)5-7(11)6-9(10)13/h5-6H,2-4H2,1H3
InchiKey: UMHZLWGUGIPASA-UHFFFAOYSA-N
Formula: C10H11Cl3O
SMILES: CCCCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 253.55

Physical Properties

Property code	Value	Unit	Source
gf	-23.95	kJ/mol	Joback Method
hf	-227.05	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	57.68	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.826		Crippen Method
mcvol	170.590	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	604.53	K	Joback Method
tc	824.93	K	Joback Method
tf	378.43	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.09	J/mol×K	604.53	Joback Method
cpg	370.66	J/mol×K	641.26	Joback Method
cpg	381.59	J/mol×K	678.00	Joback Method
cpg	391.87	J/mol×K	714.73	Joback Method
cpg	401.52	J/mol×K	751.47	Joback Method
cpg	410.55	J/mol×K	788.20	Joback Method
cpg	418.97	J/mol×K	824.93	Joback Method

dvisc	0.0010126	Pa×s	378.43	Joback Method
dvisc	0.0006633	Pa×s	416.11	Joback Method
dvisc	0.0004662	Pa×s	453.80	Joback Method
dvisc	0.0003458	Pa×s	491.48	Joback Method
dvisc	0.0002677	Pa×s	529.16	Joback Method
dvisc	0.0002144	Pa×s	566.85	Joback Method
dvisc	0.0001765	Pa×s	604.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U395218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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