

2,4,6-Trichlorobenzyl alcohol, n-propyl ether

Inchi:	InChI=1S/C10H11Cl3O/c1-2-3-14-6-8-9(12)4-7(11)5-10(8)13/h4-5H,2-3,6H2,1H3
InchiKey:	CFMBYMGVQLDZFI-UHFFFAOYSA-N
Formula:	C10H11Cl3O
SMILES:	CCCOc1c(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	-4.75		Crippen Method
logp	4.573		Crippen Method
mcvol	170.590	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinsol	1616.00		NIST Webbook
tb	604.53	K	Joback Method
tc	824.93	K	Joback Method
tf	378.43	K	Joback Method
vc	0.652	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.09	J/molxK	604.53	Joback Method
cpg	370.66	J/molxK	641.26	Joback Method
cpg	381.59	J/molxK	678.00	Joback Method
cpg	391.87	J/molxK	714.73	Joback Method
cpg	401.52	J/molxK	751.47	Joback Method
cpg	410.55	J/molxK	788.20	Joback Method
cpg	418.97	J/molxK	824.93	Joback Method
dvisc	0.0010126	Paxs	378.43	Joback Method
dvisc	0.0006633	Paxs	416.11	Joback Method

dvisc	0.0004662	Paxs	453.80	Joback Method
dvisc	0.0003458	Paxs	491.48	Joback Method
dvisc	0.0002677	Paxs	529.16	Joback Method
dvisc	0.0002144	Paxs	566.85	Joback Method
dvisc	0.0001765	Paxs	604.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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