

2,4,6-Trichlorobenzyl alcohol, neopentyl ether

Inchi:	InChI=1S/C12H15Cl3O/c1-12(2,3)7-16-6-9-10(14)4-8(13)5-11(9)15/h4-5H,6-7H2,1-3H3
InchiKey:	HKYOHTPYOYXZDV-UHFFFAOYSA-N
Formula:	C12H15Cl3O
SMILES:	CC(C)(C)COCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	281.61

Physical Properties

Property code	Value	Unit	Source
gf	-4.27	kJ/mol	Joback Method
hf	-277.08	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	60.84	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.210		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1672.00		NIST Webbook
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tb	647.06	K	Joback Method
tc	872.24	K	Joback Method
tf	403.39	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.95	J/molxK	647.06	Joback Method
cpg	472.61	J/molxK	684.59	Joback Method
cpg	485.36	J/molxK	722.12	Joback Method
cpg	497.25	J/molxK	759.65	Joback Method
cpg	508.32	J/molxK	797.18	Joback Method
cpg	518.60	J/molxK	834.71	Joback Method
cpg	528.13	J/molxK	872.24	Joback Method
dvisc	0.0009604	Paxs	403.39	Joback Method

dvisc	0.0005836	Paxs	444.00	Joback Method
dvisc	0.0003856	Paxs	484.61	Joback Method
dvisc	0.0002716	Paxs	525.22	Joback Method
dvisc	0.0002012	Paxs	565.84	Joback Method
dvisc	0.0001551	Paxs	606.45	Joback Method
dvisc	0.0001236	Paxs	647.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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