

2,4,6-Trichlorobenzyl alcohol, 2-methylbutyl ether

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

Physical Properties

Property code	Value	Unit	Source
gf	-9.55	kJ/mol	Joback Method
hf	-273.61	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.210		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	649.85	K	Joback Method
tc	866.96	K	Joback Method
tf	385.97	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.19	J/molxK	649.85	Joback Method
cpg	469.61	J/molxK	686.04	Joback Method
cpg	482.25	J/molxK	722.22	Joback Method
cpg	494.11	J/molxK	758.41	Joback Method
cpg	505.21	J/molxK	794.59	Joback Method
cpg	515.57	J/molxK	830.78	Joback Method
cpg	525.21	J/molxK	866.96	Joback Method
dvisc	0.0010834	Paxs	385.97	Joback Method

dvisc	0.0006387	Paxs	429.95	Joback Method
dvisc	0.0004154	Paxs	473.93	Joback Method
dvisc	0.0002906	Paxs	517.91	Joback Method
dvisc	0.0002150	Paxs	561.89	Joback Method
dvisc	0.0001662	Paxs	605.87	Joback Method
dvisc	0.0001330	Paxs	649.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375274&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
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

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