2,4-Dichlorobenzyl alcohol, n-pentyl ether

Other names: 2,4-dichlorobenzyl pentyl ether
Inchi: InChI=1S/C12H16Cl2O/c1-2-3-4-7-15-9-10-5-6-11(13)8-12(10)14/h5-6,8H,2-4,7,9H2,1H3
InchiKey: POIDNKWEVGRWMI-UHFFFAOYSA-N
Formula: C12H16Cl2O
SMILES: CCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 247.16

Physical Properties

Property code	Value	Unit	Source
gf	14.45	kJ/mol	Joback Method
hf	-241.12	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.700		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	607.88	K	Joback Method
tc	816.32	K	Joback Method
tf	358.53	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.18	J/mol×K	607.88	Joback Method
cpg	444.38	J/mol×K	642.62	Joback Method
cpg	457.81	J/mol×K	677.36	Joback Method
cpg	470.49	J/mol×K	712.10	Joback Method
cpg	482.43	J/mol×K	746.84	Joback Method
cpg	493.65	J/mol×K	781.58	Joback Method
cpg	504.17	J/mol×K	816.32	Joback Method
dvisc	0.0012696	Pa×s	358.53	Joback Method
dvisc	0.0007459	Pa×s	400.09	Joback Method
dvisc	0.0004843	Pa×s	441.65	Joback Method
dvisc	0.0003387	Pa×s	483.20	Joback Method
dvisc	0.0002507	Pa×s	524.76	Joback Method
dvisc	0.0001939	Pa×s	566.32	Joback Method
dvisc	0.0001554	Pa×s	607.88	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=U378111&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume