2,4-dichlorobenzyl ethyl ether

Inchi: InChI=1S/C9H10Cl2O/c1-2-12-6-7-3-4-8(10)5-9(7)11/h3-5H,2,6H2,1H3
InchiKey: KBMWRDHROVTFDI-UHFFFAOYSA-N
Formula: C9H10Cl2O
SMILES: CCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 205.08

Physical Properties

Property code	Value	Unit	Source
gf	-10.81	kJ/mol	Joback Method
hf	-179.20	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.530		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	539.24	K	Joback Method
tc	758.44	K	Joback Method
tf	324.72	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.67	J/mol×K	539.24	Joback Method
cpg	342.54	J/mol×K	721.91	Joback Method
cpg	333.37	J/mol×K	685.37	Joback Method
cpg	323.60	J/mol×K	648.84	Joback Method
cpg	313.24	J/mol×K	612.31	Joback Method
cpg	302.27	J/mol×K	575.77	Joback Method
cpg	351.13	J/mol×K	758.44	Joback Method
dvisc	0.0002037	Pa×s	539.24	Joback Method
dvisc	0.0002500	Pa×s	503.49	Joback Method
dvisc	0.0003165	Pa×s	467.73	Joback Method
dvisc	0.0004166	Pa×s	431.98	Joback Method
dvisc	0.0005763	Pa×s	396.23	Joback Method
dvisc	0.0008503	Pa×s	360.47	Joback Method
dvisc	0.0013666	Pa×s	324.72	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R32272&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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