2,4-dichlorobenzyl octyl ether

Inchi: InChI=1S/C15H22Cl2O/c1-2-3-4-5-6-7-10-18-12-13-8-9-14(16)11-15(13)17/h8-9,11H,2-7
InchiKey: XHHGKGLPLIFIEK-UHFFFAOYSA-N
Formula: C15H22Cl2O
SMILES: CCCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 289.24

Physical Properties

Property code	Value	Unit	Source
gf	39.71	kJ/mol	Joback Method
hf	-303.04	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.870		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1964.00		NIST Webbook
tb	676.52	K	Joback Method
tc	876.43	K	Joback Method
tf	392.34	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.94	J/mol×K	676.52	Joback Method
cpg	599.80	J/mol×K	709.84	Joback Method
cpg	614.79	J/mol×K	743.16	Joback Method
cpg	628.93	J/mol×K	776.47	Joback Method
cpg	642.25	J/mol×K	809.79	Joback Method
cpg	654.77	J/mol×K	843.11	Joback Method
cpg	666.50	J/mol×K	876.43	Joback Method
dvisc	0.0010807	Pa×s	392.34	Joback Method
dvisc	0.0006041	Pa×s	439.70	Joback Method
dvisc	0.0003781	Pa×s	487.07	Joback Method
dvisc	0.0002572	Pa×s	534.43	Joback Method
dvisc	0.0001862	Pa×s	581.79	Joback Method
dvisc	0.0001416	Pa×s	629.16	Joback Method
dvisc	0.0001119	Pa×s	676.52	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=R32325&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