2,4-dichlorobenzyl heptyl ether

Inchi: InChI=1S/C14H20Cl2O/c1-2-3-4-5-6-9-17-11-12-7-8-13(15)10-14(12)16/h7-8,10H,2-6,9,1
InchiKey: GQMGSURHBCAFJD-UHFFFAOYSA-N
Formula: C14H20Cl2O
SMILES: CCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 275.21

Physical Properties

Property code	Value	Unit	Source
gf	31.29	kJ/mol	Joback Method
hf	-282.40	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	61.54	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.480		Crippen Method
mcvol	214.710	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	653.64	K	Joback Method
tc	856.07	K	Joback Method
tf	381.07	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.26	J/mol×K	653.64	Joback Method
cpg	600.01	J/mol×K	822.33	Joback Method
cpg	587.86	J/mol×K	788.59	Joback Method
cpg	574.93	J/mol×K	754.85	Joback Method
cpg	561.20	J/mol×K	721.12	Joback Method
cpg	546.65	J/mol×K	687.38	Joback Method
cpg	611.41	J/mol×K	856.07	Joback Method
dvisc	0.0001255	Pa×s	653.64	Joback Method
dvisc	0.0001581	Pa×s	608.21	Joback Method
dvisc	0.0002069	Pa×s	562.78	Joback Method
dvisc	0.0002837	Pa×s	517.36	Joback Method
dvisc	0.0004134	Pa×s	471.93	Joback Method
dvisc	0.0006529	Pa×s	426.50	Joback Method
dvisc	0.0011497	Pa×s	381.07	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R32286&Units=SI

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