2,4-dichlorobenzyl hexyl ether

Inchi: InChI=1S/C13H18Cl2O/c1-2-3-4-5-8-16-10-11-6-7-12(14)9-13(11)15/h6-7,9H,2-5,8,10H2
InchiKey: RTCLSTOXGULHFW-UHFFFAOYSA-N
Formula: C13H18Cl2O
SMILES: CCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 261.19

Physical Properties

Property code	Value	Unit	Source
gf	22.87	kJ/mol	Joback Method
hf	-261.76	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.090		Crippen Method
mcvol	200.620	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1768.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	630.76	K	Joback Method
tc	836.05	K	Joback Method
tf	369.80	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.97	J/mol×K	630.76	Joback Method
cpg	546.29	J/mol×K	801.83	Joback Method
cpg	534.57	J/mol×K	767.62	Joback Method
cpg	522.10	J/mol×K	733.40	Joback Method
cpg	508.85	J/mol×K	699.19	Joback Method
cpg	494.82	J/mol×K	664.97	Joback Method
cpg	557.29	J/mol×K	836.05	Joback Method
dvisc	0.0001400	Pa×s	630.76	Joback Method
dvisc	0.0001756	Pa×s	587.27	Joback Method
dvisc	0.0002284	Pa×s	543.77	Joback Method
dvisc	0.0003110	Pa×s	500.28	Joback Method
dvisc	0.0004491	Pa×s	456.79	Joback Method
dvisc	0.0007006	Pa×s	413.29	Joback Method
dvisc	0.0012134	Pa×s	369.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R32307&Units=SI
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

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