2,4-dichlorobenzyl nonyl ether

Inchi: InChI=1S/C16H24Cl2O/c1-2-3-4-5-6-7-8-11-19-13-14-9-10-15(17)12-16(14)18/h9-10,12H
InchiKey: DVNQUGQEDVPWHU-UHFFFAOYSA-N
Formula: C16H24Cl2O
SMILES: CCCCCCCCCOCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 303.27

Physical Properties

Property code	Value	Unit	Source
gf	48.13	kJ/mol	Joback Method
hf	-323.68	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.261		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	699.40	K	Joback Method
tc	897.18	K	Joback Method
tf	403.61	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.92	J/mol×K	699.40	Joback Method
cpg	654.19	J/mol×K	732.36	Joback Method
cpg	669.56	J/mol×K	765.33	Joback Method
cpg	684.06	J/mol×K	798.29	Joback Method
cpg	697.71	J/mol×K	831.25	Joback Method
cpg	710.53	J/mol×K	864.21	Joback Method
cpg	722.56	J/mol×K	897.18	Joback Method
dvisc	0.0010085	Pa×s	403.61	Joback Method
dvisc	0.0005553	Pa×s	452.91	Joback Method
dvisc	0.0003438	Pa×s	502.21	Joback Method
dvisc	0.0002319	Pa×s	551.50	Joback Method
dvisc	0.0001668	Pa×s	600.80	Joback Method
dvisc	0.0001262	Pa×s	650.10	Joback Method
dvisc	0.0000993	Pa×s	699.40	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=R32311&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

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