

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: CCCCCCCCOCc1ccc(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	2078.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2078.00		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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