2,6-Dichlorobenzyl ether

Other names: Ether, bis(2,6-dichlorobenzyl)
Bis(2,6-dichlorobenzyl)ether
2,2',4,4'-Tetrachlorodibenzyl ether
Inchi: InChI=1S/C14H10Cl4O/c15-11-3-1-9(13(17)5-11)7-19-8-10-2-4-12(16)6-14(10)18/h1-6H
InchiKey: NWYHVMDKERUNLM-UHFFFAOYSA-N
Formula: C14H10Cl4O
SMILES: Clc1ccc(COCc2ccc(Cl)cc2Cl)c(Cl)c1
Mol. weight [g/mol]: 336.04
CAS: 73927-56-7

Physical Properties

Property code	Value	Unit	Source
gf	100.58	kJ/mol	Joback Method
hf	-100.29	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.017		Crippen Method
mcvol	215.430	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
tb	765.14	K	Joback Method
tc	1014.97	K	Joback Method
tf	492.37	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.92	J/mol×K	765.14	Joback Method
cpg	503.37	J/mol×K	806.78	Joback Method
cpg	513.82	J/mol×K	848.42	Joback Method
cpg	523.30	J/mol×K	890.05	Joback Method
cpg	531.85	J/mol×K	931.69	Joback Method
cpg	539.51	J/mol×K	973.33	Joback Method

cpg	546.32	J/mol×K	1014.97	Joback Method
dvisc	0.0005543	Pa×s	492.37	Joback Method
dvisc	0.0003736	Pa×s	537.83	Joback Method
dvisc	0.0002678	Pa×s	583.29	Joback Method
dvisc	0.0002014	Pa×s	628.76	Joback Method
dvisc	0.0001574	Pa×s	674.22	Joback Method
dvisc	0.0001269	Pa×s	719.68	Joback Method
dvisc	0.0001050	Pa×s	765.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C73927567&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume