

2-Chloro-1,4-diethoxybenzene

Inchi:	InChI=1S/C10H13ClO2/c1-3-12-8-5-6-10(13-4-2)9(11)7-8/h5-7H,3-4H2,1-2H3
InchiKey:	ZIMKMIAIVORSSX-UHFFFAOYSA-N
Formula:	C10H13ClO2
SMILES:	CCOc1ccc(OCC)c(Cl)c1
Mol. weight [g/mol]:	200.66
CAS:	52196-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-95.46	kJ/mol	Joback Method
hf	-316.32	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	50.66	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.137		Crippen Method
mvol	151.980	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1442.50		NIST Webbook
tb	547.11	K	Joback Method
tc	755.84	K	Joback Method
tf	328.30	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.16	J/molxK	547.11	Joback Method
cpg	346.25	J/molxK	581.90	Joback Method
cpg	358.76	J/molxK	616.69	Joback Method
cpg	370.66	J/molxK	651.48	Joback Method
cpg	381.96	J/molxK	686.26	Joback Method
cpg	392.65	J/molxK	721.05	Joback Method
cpg	402.73	J/molxK	755.84	Joback Method
dvisc	0.0010879	Paxs	328.30	Joback Method

dvisc	0.0006686	Paxs	364.77	Joback Method
dvisc	0.0004490	Paxs	401.24	Joback Method
dvisc	0.0003221	Paxs	437.71	Joback Method
dvisc	0.0002433	Paxs	474.17	Joback Method
dvisc	0.0001912	Paxs	510.64	Joback Method
dvisc	0.0001552	Paxs	547.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52196744&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

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