ALPHA,4-DICHLOROANISOLE

Other names: Benzene, 1-chloro-4-(chloromethoxy)-
«alpha»,4-Dichloroanisole
Inchi: InChI=1S/C7H6Cl2O/c8-5-10-7-3-1-6(9)2-4-7/h1-4H,5H2
InchiKey: PJLGIZXAYTZSIZ-UHFFFAOYSA-N
Formula: C7H6Cl2O
SMILES: ClCOc1ccc(Cl)cc1
Mol. weight [g/mol]: 177.03

Physical Properties

Property code	Value	Unit	Source
hf	-154.37	kJ/mol	Cheméo Relay (1.0)
hfus	17.12	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	2.915		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
tb	504.29	K	Cheméo Relay (1.0)
tf	313.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.37	J/mol×K	488.50	Joback Method
cpg	216.92	J/mol×K	526.11	Joback Method
cpg	225.92	J/mol×K	563.72	Joback Method
cpg	234.38	J/mol×K	601.33	Joback Method
cpg	242.31	J/mol×K	638.94	Joback Method
cpg	249.73	J/mol×K	676.55	Joback Method
cpg	256.65	J/mol×K	714.16	Joback Method
dvisc	0.0017773	Pa×s	289.66	Joback Method
dvisc	0.0010758	Pa×s	322.80	Joback Method
dvisc	0.0007150	Pa×s	355.94	Joback Method
dvisc	0.0005095	Pa×s	389.08	Joback Method

dvisc	0.0003828	Pa×s	422.22	Joback Method
dvisc	0.0002999	Pa×s	455.36	Joback Method
dvisc	0.0002428	Pa×s	488.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	2.40	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21151564&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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