4-Isopropylbenzyl chloride

Other names:	p-Isopropylbenzyl chloride
	Benzene, 1-(chloromethyl)-4-(1-methylethyl)-
	p-Cymene, 7-chloro-
	Benzene, 1-(chloromethyl)-4-(methylethyl)-
	4-Isopropylbenzyl chloride
Inchi:	InChI=1S/C10H13Cl/c1-8(2)10-5-3-9(7-11)4-6-10/h3-6,8H,7H2,1-2H3
InchiKey:	CYAKWEQUWJAHLW-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CC(C)c1ccc(CCl)cc1
Mol. weight [g/mol]:	168.67

Physical Properties

Property code	Value	Unit	Source
af	0.3917		Cheméo Relay (1.0)
gf	121.73	kJ/mol	Joback Method
hf	-84.31	kJ/mol	Cheméo Relay (1.0)
hfus	15.98	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-4.38		Cheméo Relay (1.0)
logp	3.549		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	502.61	K	Cheméo Relay (1.0)
tc	720.33	K	Cheméo Relay (1.0)
tf	289.20	K	Cheméo Relay (1.0)
vc	0.506	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.81	J/mol×K	496.85	Joback Method

cpg	360.16	J/mol×K	713.53	Joback Method
cpg	349.64	J/mol×K	677.42	Joback Method
cpg	338.41	J/mol×K	641.30	Joback Method
cpg	326.45	J/mol×K	605.19	Joback Method
cpg	313.72	J/mol×K	569.08	Joback Method
cpg	300.18	J/mol×K	532.96	Joback Method
dvisc	0.0005590	Pa×s	376.58	Joback Method
dvisc	0.0002211	Pa×s	496.85	Joback Method
dvisc	0.0002853	Pa×s	456.76	Joback Method
dvisc	0.0003866	Pa×s	416.67	Joback Method
dvisc	0.0033760	Pa×s	256.32	Joback Method
dvisc	0.0008825	Pa×s	336.50	Joback Method
dvisc	0.0015764	Pa×s	296.41	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051185&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

af: Acentric Factor
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
ie: Ionization energy
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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