

4-Methoxy-3-methylbenzyl chloride

Inchi:	InChI=1S/C9H11ClO/c1-7-5-8(6-10)3-4-9(7)11-2/h3-5H,6H2,1-2H3
InchiKey:	BHEHNICAPZVKRH-UHFFFAOYSA-N
Formula:	C9H11ClO
SMILES:	COc1ccc(CCl)cc1C
Mol. weight [g/mol]:	170.64
CAS:	60736-71-2

Physical Properties

Property code	Value	Unit	Source
gf	1.12	kJ/mol	Joback Method
hf	-163.46	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.742		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	501.81	K	Joback Method
tc	716.06	K	Joback Method
tf	294.80	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.84	J/molxK	501.81	Joback Method
cpg	321.16	J/molxK	680.35	Joback Method
cpg	311.25	J/molxK	644.64	Joback Method
cpg	300.76	J/molxK	608.93	Joback Method
cpg	289.71	J/molxK	573.23	Joback Method
cpg	278.07	J/molxK	537.52	Joback Method
cpg	330.52	J/molxK	716.06	Joback Method
dvisc	0.0002004	Paxs	501.81	Joback Method
dvisc	0.0002456	Paxs	467.31	Joback Method

dvisc	0.0003109	Paxs	432.81	Joback Method
dvisc	0.0004100	Paxs	398.31	Joback Method
dvisc	0.0005698	Paxs	363.80	Joback Method
dvisc	0.0008484	Paxs	329.30	Joback Method
dvisc	0.0013866	Paxs	294.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60736712&Units=SI

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

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