1-Chloromethyl-3,5-dimethylbenzene

Other names: Benzene,1-(chloromethyl)-3,5-dimethyl-
3,5-Dimethylbenzyl chloride
Inchi: InChI=1S/C9H11Cl/c1-7-3-8(2)5-9(4-7)6-10/h3-5H,6H2,1-2H3
InchiKey: FYNVRRYQTHUESZ-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: Cc1cc(C)cc(CCl)c1
Mol. weight [g/mol]: 154.64
CAS: 2745-54-2

Physical Properties

Property code	Value	Unit	Source
gf	106.12	kJ/mol	Joback Method
hf	-31.24	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
ie	8.63 ± 0.03	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	3.042		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1196.00		NIST Webbook
tb	479.39	K	Joback Method
tc	695.70	K	Joback Method
tf	272.57	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.19	J/mol×K	479.39	Joback Method
cpg	255.67	J/mol×K	515.44	Joback Method
cpg	267.48	J/mol×K	551.49	Joback Method
cpg	278.64	J/mol×K	587.55	Joback Method
cpg	289.18	J/mol×K	623.60	Joback Method

cpg	299.10	J/mol×K	659.65	Joback Method
cpg	308.45	J/mol×K	695.70	Joback Method
dvisc	0.0017313	Pa×s	272.57	Joback Method
dvisc	0.0010303	Pa×s	307.04	Joback Method
dvisc	0.0006809	Pa×s	341.51	Joback Method
dvisc	0.0004855	Pa×s	375.98	Joback Method
dvisc	0.0003664	Pa×s	410.45	Joback Method
dvisc	0.0002888	Pa×s	444.92	Joback Method
dvisc	0.0002356	Pa×s	479.39	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2745542&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
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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