1-Chloro-3-isopropyl-4-methylbenzene

Inchi: InChI=1S/C10H13Cl/c1-7(2)10-6-9(11)5-4-8(10)3/h4-7H,1-3H3
InchiKey: ISPBEETWYSGCDQ-UHFFFAOYSA-N
Formula: C10H13Cl
SMILES: Cc1ccc(Cl)cc1C(C)C
Mol. weight [g/mol]: 168.66
CAS: 63831-93-6

Physical Properties

Property code	Value	Unit	Source
gf	112.10	kJ/mol	Joback Method
hf	-57.16	kJ/mol	Joback Method
hfl	-108.00 ± 4.50	kJ/mol	NIST Webbook
hfus	15.59	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.772		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	501.83	K	Joback Method
tc	719.75	K	Joback Method
tf	268.84	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.03	J/mol×K	501.83	Joback Method
cpg	348.45	J/mol×K	683.43	Joback Method
cpg	337.40	J/mol×K	647.11	Joback Method
cpg	325.66	J/mol×K	610.79	Joback Method
cpg	313.20	J/mol×K	574.47	Joback Method
cpg	300.00	J/mol×K	538.15	Joback Method
cpg	358.83	J/mol×K	719.75	Joback Method
dvisc	0.0002130	Pa×s	501.83	Joback Method

dvisc	0.0002688	Pa×s	463.00	Joback Method
dvisc	0.0003540	Pa×s	424.17	Joback Method
dvisc	0.0004928	Pa×s	385.34	Joback Method
dvisc	0.0007387	Pa×s	346.50	Joback Method
dvisc	0.0012266	Pa×s	307.67	Joback Method
dvisc	0.0023579	Pa×s	268.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63831936&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
hfl:	Liquid phase 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