

1-Chloro-2-isopropyl-4-methylbenzene

Inchi:	InChI=1S/C10H13Cl/c1-7(2)9-6-8(3)4-5-10(9)11/h4-7H,1-3H3
InchiKey:	ZYHNYRQDNMFBW-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	Cc1ccc(Cl)c(C(C)C)c1
Mol. weight [g/mol]:	168.66
CAS:	15146-00-6

Physical Properties

Property code	Value	Unit	Source
gf	112.10	kJ/mol	Joback Method
hf	-57.16	kJ/mol	Joback Method
hfl	-111.60 ± 2.20	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.03	J/mol×K	501.83	Joback Method
cpg	300.00	J/mol×K	538.15	Joback Method
cpg	313.20	J/mol×K	574.47	Joback Method
cpg	325.66	J/mol×K	610.79	Joback Method
cpg	337.40	J/mol×K	647.11	Joback Method
cpg	348.45	J/mol×K	683.43	Joback Method
cpg	358.83	J/mol×K	719.75	Joback Method
dvisc	0.0023579	Paxs	268.84	Joback Method

dvisc	0.0012266	Paxs	307.67	Joback Method
dvisc	0.0007387	Paxs	346.50	Joback Method
dvisc	0.0004928	Paxs	385.34	Joback Method
dvisc	0.0003540	Paxs	424.17	Joback Method
dvisc	0.0002688	Paxs	463.00	Joback Method
dvisc	0.0002130	Paxs	501.83	Joback Method
hvapt	47.10	kJ/mol	445.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15146006&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
hvapt:	Enthalpy of vaporization at a given temperature
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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