

1-Chloro-3,5-diisopropylbenzene

Inchi:	InChI=1S/C12H17Cl/c1-8(2)10-5-11(9(3)4)7-12(13)6-10/h5-9H,1-4H3
InchiKey:	IJPBANLIWUXUPV-UHFFFAOYSA-N
Formula:	C12H17Cl
SMILES:	CC(C)c1cc(Cl)cc(C(C)C)c1
Mol. weight [g/mol]:	196.72
CAS:	87945-06-0

Physical Properties

Property code	Value	Unit	Source
gf	126.50	kJ/mol	Joback Method
hf	-103.72	kJ/mol	Joback Method
hfl	170.00 ± 4.20	kJ/mol	NIST Webbook
hfus	17.25	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.587		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	547.15	K	Joback Method
tc	762.69	K	Joback Method
tf	276.38	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.33	J/molxK	547.15	Joback Method
cpg	393.50	J/molxK	583.07	Joback Method
cpg	408.76	J/molxK	619.00	Joback Method
cpg	423.15	J/molxK	654.92	Joback Method
cpg	436.70	J/molxK	690.85	Joback Method
cpg	449.44	J/molxK	726.77	Joback Method
cpg	461.40	J/molxK	762.69	Joback Method
dvisc	0.0031791	Paxs	276.38	Joback Method

dvisc	0.0013976	Paxs	321.51	Joback Method
dvisc	0.0007522	Paxs	366.64	Joback Method
dvisc	0.0004637	Paxs	411.76	Joback Method
dvisc	0.0003145	Paxs	456.89	Joback Method
dvisc	0.0002288	Paxs	502.02	Joback Method
dvisc	0.0001754	Paxs	547.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87945060&Units=SI
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

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

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