1-Chloro-2,5-diisopropylbenzene

Inchi: InChI=1S/C12H17Cl/c1-8(2)10-5-6-11(9(3)4)12(13)7-10/h5-9H,1-4H3
InchiKey: DAQRAOORRPJOKE-UHFFFAOYSA-N
Formula: C12H17Cl
SMILES: CC(C)c1ccc(C(C)C)c(Cl)c1
Mol. weight [g/mol]: 196.72
CAS: 49841-53-4

Physical Properties

Property code	Value	Unit	Source
gf	126.50	kJ/mol	Joback Method
hf	-103.72	kJ/mol	Joback Method
hfl	-165.00 ± 3.30	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/mol×K	547.15	Joback Method
cpg	449.44	J/mol×K	726.77	Joback Method
cpg	436.70	J/mol×K	690.85	Joback Method
cpg	423.15	J/mol×K	654.92	Joback Method
cpg	408.76	J/mol×K	619.00	Joback Method
cpg	393.50	J/mol×K	583.07	Joback Method
cpg	461.40	J/mol×K	762.69	Joback Method
dvisc	0.0001754	Pa×s	547.15	Joback Method

dvisc	0.0002288	Pa×s	502.02	Joback Method
dvisc	0.0003145	Pa×s	456.89	Joback Method
dvisc	0.0004637	Pa×s	411.76	Joback Method
dvisc	0.0007522	Pa×s	366.64	Joback Method
dvisc	0.0013976	Pa×s	321.51	Joback Method
dvisc	0.0031791	Pa×s	276.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C49841534&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