

1-Chloro-3-[1-(4-chlorophenyl)ethyl]benzene

Inchi:	InChI=1S/C14H12Cl2/c1-10(11-5-7-13(15)8-6-11)12-3-2-4-14(16)9-12/h2-10H,1H3
InchiKey:	RCBXKRCNRRAKLO-UHFFFAOYSA-N
Formula:	C14H12Cl2
SMILES:	CC(c1ccc(Cl)cc1)c1cccc(Cl)c1
Mol. weight [g/mol]:	251.15
CAS:	77008-64-1

Physical Properties

Property code	Value	Unit	Source
gf	246.26	kJ/mol	Joback Method
hf	81.07	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	61.02	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.145		Crippen Method
mcvol	185.080	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	657.46	K	Joback Method
tc	910.84	K	Joback Method
tf	370.26	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.34	J/molxK	657.46	Joback Method
cpg	440.27	J/molxK	699.69	Joback Method
cpg	453.96	J/molxK	741.92	Joback Method
cpg	466.50	J/molxK	784.15	Joback Method
cpg	477.97	J/molxK	826.38	Joback Method
cpg	488.45	J/molxK	868.61	Joback Method
cpg	498.01	J/molxK	910.84	Joback Method
dvisc	0.0015430	Paxs	370.26	Joback Method
dvisc	0.0008383	Paxs	418.13	Joback Method

dvisc	0.0005162	Paxs	465.99	Joback Method
dvisc	0.0003479	Paxs	513.86	Joback Method
dvisc	0.0002508	Paxs	561.73	Joback Method
dvisc	0.0001904	Paxs	609.59	Joback Method
dvisc	0.0001504	Paxs	657.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77008641&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
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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