4-(CH2Cl)-C6H4-CN

Other names: 3-Cyanobenzylchloride
4-(CH2Cl)-C6H4-CN
4-(chloromethyl)benzonitrile
Inchi: InChI=1S/C8H6ClN/c9-5-7-1-3-8(6-10)4-2-7/h1-4H,5H2
InchiKey: LOQLDQJTSMKBJU-UHFFFAOYSA-N
Formula: C8H6ClN
SMILES: N#Cc1ccc(CCl)cc1
Mol. weight [g/mol]: 151.60

Physical Properties

Property code	Value	Unit	Source
af	0.4412		Cheméo Relay (1.0)
affp	812.80	kJ/mol	NIST Webbook
basg	782.10	kJ/mol	NIST Webbook
gf	240.51	kJ/mol	Joback Method
hf	129.94	kJ/mol	Cheméo Relay (1.0)
hfus	15.83	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.297		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	527.16	K	Cheméo Relay (1.0)
tc	769.28	K	Cheméo Relay (1.0)
tf	340.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.76	J/mol×K	553.61	Joback Method
cpg	232.04	J/mol×K	593.20	Joback Method
cpg	240.67	J/mol×K	632.78	Joback Method
cpg	248.68	J/mol×K	672.37	Joback Method

cpg	256.09	J/mol×K	711.95	Joback Method
cpg	262.95	J/mol×K	751.54	Joback Method
cpg	269.27	J/mol×K	791.13	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C874862&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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