

3,4-DICHLOROPHENYLACETONITRILE

Other names:	3,4-Dichlorobenzyl cyanide Benzeneacetonitrile, 3,4-dichloro-
Inchi:	InChI=1S/C8H5Cl2N/c9-7-2-1-6(3-4-11)5-8(7)10/h1-2,5H,3H2
InchiKey:	QWZNCAFWRZZJMA-UHFFFAOYSA-N
Formula:	C8H5Cl2N
SMILES:	N#CCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	186.04

Physical Properties

Property code	Value	Unit	Source
hfus	19.64	kJ/mol	Joback Method
hvap	75.52	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
logp	3.059		Crippen Method
mcvol	125.680	ml/mol	McGowan Method
tb	547.43	K	Cheméo Relay (1.0)
tf	330.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.66	J/mol×K	596.02	Joback Method
cpg	249.88	J/mol×K	636.43	Joback Method
cpg	257.50	J/mol×K	676.83	Joback Method
cpg	264.56	J/mol×K	717.24	Joback Method
cpg	271.08	J/mol×K	757.64	Joback Method
cpg	277.09	J/mol×K	798.05	Joback Method
cpg	282.61	J/mol×K	838.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3218493&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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