Benzamide, 2,5-dichloro-n-cyanomethyl-3-nitro-

Inchi: InChI=1S/C9H5Cl2N3O3/c10-5-3-6(9(15)13-2-1-12)8(11)7(4-5)14(16)17/h3-4H,2H2,(H,1

InchiKey: SCHAPWDTKXLDEP-UHFFFAOYSA-N

Formula: C9H5Cl2N3O3

SMILES: N#CCNC(=O)c1cc(Cl)cc([N+](=O)[O-])c1Cl

Mol. weight [g/mol]: 274.06

CAS: 22978-18-3

Physical Properties

Property code	Value	Unit	Source
gf	213.76	kJ/mol	Joback Method
hf	36.56	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	2.155		Crippen Method
mcvol	168.740	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	879.76	K	Joback Method
tc	1137.44	K	Joback Method
tf	626.20	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.46	J/mol×K	879.76	Joback Method
cpg	411.70	J/mol×K	922.71	Joback Method
cpg	417.23	J/mol×K	965.65	Joback Method
cpg	422.08	J/mol×K	1008.60	Joback Method
cpg	426.29	J/mol×K	1051.54	Joback Method
cpg	429.91	J/mol×K	1094.49	Joback Method
cpg	432.96	J/mol×K	1137.44	Joback Method

Sources

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=C22978183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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