Phenylsuccinonitrile

Inchi: InChI=1S/C10H8N2/c11-7-6-10(8-12)9-4-2-1-3-5-9/h1-5,10H,6H2
InchiKey: PERNOSOTUDEXCY-UHFFFAOYSA-N
Formula: C10H8N2
SMILES: N#CCC(C#N)c1ccccc1
Mol. weight [g/mol]: 156.18
CAS: 13706-68-8

Physical Properties

Property code	Value	Unit	Source
gf	409.65	kJ/mol	Joback Method
hf	311.28	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.207		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	658.60	K	Joback Method
tc	900.79	K	Joback Method
tf	343.86	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.09	J/mol×K	658.60	Joback Method
cpg	317.10	J/mol×K	698.97	Joback Method
cpg	326.32	J/mol×K	739.33	Joback Method
cpg	334.81	J/mol×K	779.70	Joback Method
cpg	342.60	J/mol×K	820.06	Joback Method
cpg	349.75	J/mol×K	860.43	Joback Method
cpg	356.31	J/mol×K	900.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.50 ± 2.50	K	0.07	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13706688&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume