O-ETHYLBENZONITRILE

Inchi: InChI=1S/C9H9N/c1-2-8-5-3-4-6-9(8)7-10/h3-6H,2H2,1H3
InchiKey: UZDXATQPJOOHQJ-UHFFFAOYSA-N
Formula: C9H9N
SMILES: CCc1ccccc1C#N
Mol. weight [g/mol]: 131.18

Physical Properties

Property code	Value	Unit	Source
af	0.4178		Cheméo Relay (1.0)
gf	260.86	kJ/mol	Joback Method
hf	150.17	kJ/mol	Cheméo Relay (1.0)
hfus	14.22	kJ/mol	Joback Method
hvap	60.47	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	2.121		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	502.96	K	Cheméo Relay (1.0)
tc	729.29	K	Cheméo Relay (1.0)
tf	250.90	K	Cheméo Relay (1.0)
vc	0.417	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.50	J/mol×K	539.06	Joback Method
cpg	254.71	J/mol×K	577.16	Joback Method
cpg	265.21	J/mol×K	615.26	Joback Method
cpg	275.04	J/mol×K	653.35	Joback Method
cpg	284.23	J/mol×K	691.45	Joback Method
cpg	292.80	J/mol×K	729.55	Joback Method
cpg	300.78	J/mol×K	767.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34136599&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
vc:	Critical Volume