4,4-Ethylenedioxy-pentanenitrile

Other names: 1,3-dioxolane-2-propanenitrile, 2-methyl-
Inchi: InChI=1S/C7H11NO2/c1-7(3-2-4-8)9-5-6-10-7/h2-3,5-6H2,1H3
InchiKey: WAKYIWZYFCUCSG-UHFFFAOYSA-N
Formula: C7H11NO2
SMILES: CC1(CCC#N)OCCO1
Mol. weight [g/mol]: 141.17
CAS: 40159-07-7

Physical Properties

Property code	Value	Unit	Source
gf	0.06	kJ/mol	Joback Method
hf	-211.21	kJ/mol	Joback Method
hfus	18.99	kJ/mol	Joback Method
hvap	49.78	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.053		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	531.06	K	Joback Method
tc	755.31	K	Joback Method
tf	321.58	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.58	J/mol×K	531.06	Joback Method
cpg	279.46	J/mol×K	568.43	Joback Method
cpg	290.49	J/mol×K	605.81	Joback Method
cpg	300.81	J/mol×K	643.18	Joback Method
cpg	310.53	J/mol×K	680.56	Joback Method
cpg	319.78	J/mol×K	717.93	Joback Method
cpg	328.67	J/mol×K	755.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40159077&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume