

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

Physical Properties

Property code	Value	Unit	Source
hfus	18.99	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Cheméo Relay (1.0)
logp	1.053		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
tb	499.13	K	Cheméo Relay (1.0)
tf	276.27	K	Cheméo Relay (1.0)

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

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):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40159077&Units=SI>

Legend

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

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