

2-ethylbutanenitrile

Inchi:	InChI=1S/C6H11N/c1-3-6(4-2)5-7/h6H,3-4H2,1-2H3
InchiKey:	QARLTYSAFQGMMB-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	CCC(C#N)CC
Mol. weight [g/mol]:	97.16
CAS:	617-80-1

Physical Properties

Property code	Value	Unit	Source
hf	-7.64	kJ/mol	Cheméo Relay (1.0)
hfus	9.28	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Cheméo Relay (1.0)
logp	1.946		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
tb	419.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.99	J/mol×K	438.32	Joback Method
cpg	199.58	J/mol×K	470.54	Joback Method
cpg	208.77	J/mol×K	502.76	Joback Method
cpg	217.55	J/mol×K	534.97	Joback Method
cpg	225.93	J/mol×K	567.19	Joback Method
cpg	233.94	J/mol×K	599.41	Joback Method
cpg	241.57	J/mol×K	631.63	Joback Method

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45778e+01
Coeff. B	-3.58148e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	308.02
Temperature range (K), max.	443.90

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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