PROPANAL, 3-CYANO-

Other names: Propanal, 3-cyano-
«beta»-Cyanopropionaldehyde
3-formylpropiononitrile
Inchi: InChI=1S/C4H5NO/c5-3-1-2-4-6/h4H,1-2H2
InchiKey: CGFGIKNLZTZJDE-UHFFFAOYSA-N
Formula: C4H5NO
SMILES: N#CCCC=O
Mol. weight [g/mol]: 83.09

Physical Properties

Property code	Value	Unit	Source
chl	-2301.50 ± 1.50	kJ/mol	NIST Webbook
hf	-26.25	kJ/mol	Cheméo Relay (1.0)
hfl	12.80 ± 1.50	kJ/mol	NIST Webbook
hfus	9.91	kJ/mol	Joback Method
ie	11.14	eV	Cheméo Relay (1.0)
logp	0.489		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
tb	455.19	K	Cheméo Relay (1.0)
tf	265.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.12	J/mol×K	441.66	Joback Method
cpg	134.70	J/mol×K	474.85	Joback Method
cpg	140.02	J/mol×K	508.05	Joback Method
cpg	145.09	J/mol×K	541.24	Joback Method
cpg	149.92	J/mol×K	574.43	Joback Method
cpg	154.51	J/mol×K	607.62	Joback Method
cpg	158.86	J/mol×K	640.82	Joback Method
cpl	195.90	J/mol×K	300.00	NIST Webbook

Sources

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=C3515933&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point