

6-Heptene-1-nitrile

Other names:	(Replicate of what you have as 6-Cyano-1-hexene)
Inchi:	InChI=1S/C7H11N/c1-2-3-4-5-6-7-8/h2H,1,3-6H2
InchiKey:	ZLWQKLRLMIQIHKQ-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	C=CCCCCC#N
Mol. weight [g/mol]:	109.17
CAS:	5048-25-9

Physical Properties

Property code	Value	Unit	Source
gf	229.08	kJ/mol	Joback Method
hf	102.50	kJ/mol	Joback Method
hfus	14.11	kJ/mol	Joback Method
hvap	40.98	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.256		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	458.32	K	Joback Method
tc	649.32	K	Joback Method
tf	231.88	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.73	J/mol×K	458.32	Joback Method
cpg	222.56	J/mol×K	490.15	Joback Method
cpg	231.93	J/mol×K	521.99	Joback Method
cpg	240.86	J/mol×K	553.82	Joback Method
cpg	249.36	J/mol×K	585.65	Joback Method
cpg	257.46	J/mol×K	617.48	Joback Method
cpg	265.15	J/mol×K	649.32	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5048259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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