

2-Heptynoic acid

Other names:	hept-2-ynoic acid
Inchi:	InChI=1S/C7H10O2/c1-2-3-4-5-6-7(8)9/h2-4H2,1H3,(H,8,9)
InchiKey:	UEERQXQKEJPYBR-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CCCCC#CC(=O)O
Mol. weight [g/mol]:	126.15
CAS:	1483-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-54.88	kJ/mol	Joback Method
hf	-180.32	kJ/mol	Joback Method
hfus	22.70	kJ/mol	Joback Method
hvap	56.75	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.265		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	514.61	K	Joback Method
tc	705.50	K	Joback Method
tf	385.50	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.74	J/mol×K	514.61	Joback Method
cpg	239.50	J/mol×K	546.42	Joback Method
cpg	247.87	J/mol×K	578.24	Joback Method
cpg	255.87	J/mol×K	610.05	Joback Method
cpg	263.49	J/mol×K	641.87	Joback Method
cpg	270.76	J/mol×K	673.68	Joback Method
cpg	277.69	J/mol×K	705.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57124e+01
Coeff. B	-5.01495e+03
Coeff. C	-9.25450e+01
Temperature range (K), min.	418.15
Temperature range (K), max.	575.15

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=C1483676&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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