

2-Nonynoic acid, methyl ester

Other names:	Methyl 2-nonynoate 1-Octynecarboxylic acid, methyl ester methyl non-2-ynoate
Inchi:	InChI=1S/C10H16O2/c1-3-4-5-6-7-8-9-10(11)12-2/h3-7H2,1-2H3
InchiKey:	NTLJTUMJJWVCTL-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CCCCCCC#CC(=O)OC
Mol. weight [g/mol]:	168.23
CAS:	111-80-8

Physical Properties

Property code	Value	Unit	Source
gf	2.20	kJ/mol	Joback Method
hf	-222.23	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.133		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1311.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	513.49	K	Joback Method
tc	707.09	K	Joback Method
tf	380.72	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	334.69	J/mol×K	513.49	Joback Method
cpg	348.11	J/mol×K	545.76	Joback Method
cpg	361.00	J/mol×K	578.02	Joback Method
cpg	373.34	J/mol×K	610.29	Joback Method
cpg	385.15	J/mol×K	642.55	Joback Method
cpg	396.44	J/mol×K	674.82	Joback Method
cpg	407.19	J/mol×K	707.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	2.70	NIST Webbook
tbrp	358.20	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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