4-Methyl-nonanal

Other names: 4-methylnonan-1-al
Inchi: InChI=1S/C10H20O/c1-3-4-5-7-10(2)8-6-9-11/h9-10H,3-8H2,1-2H3
InchiKey: DHBWTBZYMOTKID-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCCCCC(C)CCC=O
Mol. weight [g/mol]: 156.27
CAS: 94088-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-68.64	kJ/mol	Joback Method
hf	-340.59	kJ/mol	Joback Method
hfus	20.42	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1155.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1429.00		NIST Webbook
tb	476.42	K	Joback Method
tc	648.48	K	Joback Method
tf	229.46	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.77	J/mol×K	476.42	Joback Method
cpg	357.21	J/mol×K	505.10	Joback Method
cpg	371.06	J/mol×K	533.77	Joback Method

cpg	384.34	J/mol×K	562.45	Joback Method
cpg	397.06	J/mol×K	591.13	Joback Method
cpg	409.23	J/mol×K	619.81	Joback Method
cpg	420.88	J/mol×K	648.48	Joback Method
dvisc	0.0078468	Pa×s	229.46	Joback Method
dvisc	0.0029372	Pa×s	270.62	Joback Method
dvisc	0.0014251	Pa×s	311.78	Joback Method
dvisc	0.0008185	Pa×s	352.94	Joback Method
dvisc	0.0005278	Pa×s	394.10	Joback Method
dvisc	0.0003698	Pa×s	435.26	Joback Method
dvisc	0.0002756	Pa×s	476.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94088309&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume