

Neodecanoic acid

Other names:	Wiltz-65
Inchi:	InChI=1S/C10H20O2/c1-4-5-6-7-8-10(2,3)9(11)12/h4-8H2,1-3H3,(H,11,12)
InchiKey:	IKNDGHRNXGEHTO-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCC(C)(C)C(=O)O
Mol. weight [g/mol]:	172.26
CAS:	26896-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-229.58	kJ/mol	Joback Method
hf	-523.29	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	3.068		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	571.02	K	Joback Method
tc	746.12	K	Joback Method
tf	315.63	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.06	J/mol×K	571.02	Joback Method
cpg	465.12	J/mol×K	716.93	Joback Method
cpg	454.49	J/mol×K	687.75	Joback Method
cpg	443.30	J/mol×K	658.57	Joback Method
cpg	431.51	J/mol×K	629.39	Joback Method
cpg	419.11	J/mol×K	600.20	Joback Method
cpg	475.22	J/mol×K	746.12	Joback Method
dvisc	0.0000963	Pa×s	571.02	Joback Method

dvisc	0.0001568	Pa×s	528.45	Joback Method
dvisc	0.0002781	Pa×s	485.89	Joback Method
dvisc	0.0005509	Pa×s	443.32	Joback Method
dvisc	0.0012615	Pa×s	400.76	Joback Method
dvisc	0.0035176	Pa×s	358.19	Joback Method
dvisc	0.0129334	Pa×s	315.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26896208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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