

Decanoyl chloride

Other names:	n-Decanoyl chloride Caprinoyl chloride Capric acid chloride
Inchi:	InChI=1S/C10H19ClO/c1-2-3-4-5-6-7-8-9-10(11)12/h2-9H2,1H3
InchiKey:	IPIVAXLHTVNRBS-UHFFFAOYSA-N
Formula:	C10H19ClO
SMILES:	CCCCCCCCC(=O)Cl
Mol. weight [g/mol]:	190.71
CAS:	112-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-107.53	kJ/mol	Joback Method
hf	-378.05	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.892		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinsol	1316.40		NIST Webbook
tb	519.50	K	Joback Method
tc	697.68	K	Joback Method
tf	282.31	K	Joback Method
vc	0.650	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.80	J/mol×K	519.50	Joback Method
cpg	386.68	J/mol×K	549.20	Joback Method
cpg	399.94	J/mol×K	578.89	Joback Method
cpg	412.62	J/mol×K	608.59	Joback Method
cpg	424.72	J/mol×K	638.29	Joback Method

cpg	436.27	J/molxK	667.99	Joback Method
cpg	447.28	J/molxK	697.68	Joback Method
dvisc	0.0040367	Paxs	282.31	Joback Method
dvisc	0.0019523	Paxs	321.84	Joback Method
dvisc	0.0011069	Paxs	361.37	Joback Method
dvisc	0.0007019	Paxs	400.90	Joback Method
dvisc	0.0004830	Paxs	440.44	Joback Method
dvisc	0.0003535	Paxs	479.97	Joback Method
dvisc	0.0002713	Paxs	519.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	0.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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