Hexanoyl chloride, 3,5,5-trimethyl-

Other names: 3,5,5-Trimethylhexanoyl chloride
Inchi: InChI=1S/C9H17ClO/c1-7(5-8(10)11)6-9(2,3)4/h7H,5-6H2,1-4H3
InchiKey: GEKPNPPFAYJZRD-UHFFFAOYSA-N
Formula: C9H17ClO
SMILES: CC(CC(=O)Cl)CC(C)(C)C
Mol. weight [g/mol]: 176.68
CAS: 36727-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-115.55	kJ/mol	Joback Method
hf	-371.44	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.214		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
tb	492.95	K	Joback Method
tc	687.99	K	Joback Method
tf	258.46	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.57	J/mol×K	492.95	Joback Method
cpg	395.27	J/mol×K	655.48	Joback Method
cpg	383.79	J/mol×K	622.98	Joback Method
cpg	371.61	J/mol×K	590.47	Joback Method
cpg	358.71	J/mol×K	557.96	Joback Method
cpg	345.04	J/mol×K	525.46	Joback Method

cpg	406.08	J/mol×K	687.99	Joback Method
dvisc	0.0002716	Pa×s	492.95	Joback Method
dvisc	0.0003755	Pa×s	453.87	Joback Method
dvisc	0.0005517	Pa×s	414.79	Joback Method
dvisc	0.0008783	Pa×s	375.70	Joback Method
dvisc	0.0015574	Pa×s	336.62	Joback Method
dvisc	0.0032103	Pa×s	297.54	Joback Method
dvisc	0.0082353	Pa×s	258.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36727294&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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