3,5,5-Trimethylhexanoyl chloride

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]: 176.69

Physical Properties

Property code	Value	Unit	Source
af	0.4194		Cheméo Relay (1.0)
gf	-115.55	kJ/mol	Joback Method
hf	-429.83	kJ/mol	Cheméo Relay (1.0)
hfus	13.93	kJ/mol	Joback Method
hvap	46.78	kJ/mol	Cheméo Relay (1.0)
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	453.16	K	Cheméo Relay (1.0)
tc	630.79	K	Cheméo Relay (1.0)
tf	239.90	K	Cheméo Relay (1.0)
vc	0.517	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.57	J/mol×K	492.95	Joback Method
cpg	406.08	J/mol×K	687.99	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

dvisc	0.0008783	Pa×s	375.71	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	0.0082353	Pa×s	258.46	Joback Method
dvisc	0.0015574	Pa×s	336.62	Joback Method
dvisc	0.0032103	Pa×s	297.54	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36727294&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
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