2,7-DIMETHYLOCTAN-4-ONE

Inchi: InChI=1S/C10H20O/c1-8(2)5-6-10(11)7-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey: FSDBXGZREACSJJ-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CC(C)CCC(=O)CC(C)C
Mol. weight [g/mol]: 156.27

Physical Properties

Property code	Value	Unit	Source
af	0.4867		Cheméo Relay (1.0)
hf	-393.01	kJ/mol	Cheméo Relay (1.0)
hfus	16.21	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	3.038		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
tb	470.00 ± 4.00	K	NIST Webbook
tc	638.72	K	Cheméo Relay (1.0)
tf	255.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.29	J/mol×K	481.19	Joback Method
cpg	357.47	J/mol×K	511.21	Joback Method
cpg	372.01	J/mol×K	541.23	Joback Method
cpg	385.92	J/mol×K	571.24	Joback Method
cpg	399.22	J/mol×K	601.26	Joback Method
cpg	411.92	J/mol×K	631.28	Joback Method
cpg	424.04	J/mol×K	661.30	Joback Method
dvisc	0.0108635	Pa×s	222.39	Joback Method
dvisc	0.0034410	Pa×s	265.52	Joback Method
dvisc	0.0015030	Pa×s	308.66	Joback Method

dvisc	0.0008043	Pa×s	351.79	Joback Method
dvisc	0.0004934	Pa×s	394.92	Joback Method
dvisc	0.0003333	Pa×s	438.06	Joback Method
dvisc	0.0002415	Pa×s	481.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C59387927&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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