Methyl-2,6-Dimethyl-5-oxoheptanoate

Inchi: InChI=1S/C10H18O3/c1-7(2)9(11)6-5-8(3)10(12)13-4/h7-8H,5-6H2,1-4H3
InchiKey: UDVSCIOUANKHJU-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: COC(=O)C(C)CCC(=O)C(C)C
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-334.40	kJ/mol	Joback Method
hf	-617.67	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.801		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1243.00		NIST Webbook
tb	557.48	K	Joback Method
tc	745.50	K	Joback Method
tf	294.55	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.89	J/mol×K	557.48	Joback Method
cpg	454.64	J/mol×K	714.16	Joback Method
cpg	443.11	J/mol×K	682.83	Joback Method
cpg	430.98	J/mol×K	651.49	Joback Method
cpg	418.24	J/mol×K	620.15	Joback Method
cpg	404.87	J/mol×K	588.82	Joback Method
cpg	465.56	J/mol×K	745.50	Joback Method
dvisc	0.0002082	Pa×s	557.48	Joback Method
dvisc	0.0002802	Pa×s	513.66	Joback Method

dvisc	0.0003987	Pa×s	469.84	Joback Method
dvisc	0.0006100	Pa×s	426.01	Joback Method
dvisc	0.0010288	Pa×s	382.19	Joback Method
dvisc	0.0019868	Pa×s	338.37	Joback Method
dvisc	0.0046668	Pa×s	294.55	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R229306&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