6-p-Tolylheptan-2-one

Inchi: InChI=1S/C14H20O/c1-11-7-9-14(10-8-11)12(2)5-4-6-13(3)15/h7-10,12H,4-6H2,1-3H3
InchiKey: URMNPIAGMIVNMU-UHFFFAOYSA-N
Formula: C14H20O
SMILES: CC(=O)CCCC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	38.42	kJ/mol	Joback Method
hf	-225.09	kJ/mol	Joback Method
hfus	23.74	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.858		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2211.00		NIST Webbook
tb	604.81	K	Joback Method
tc	811.67	K	Joback Method
tf	321.41	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.19	J/mol×K	604.81	Joback Method
cpg	484.06	J/mol×K	639.29	Joback Method
cpg	499.97	J/mol×K	673.76	Joback Method
cpg	514.95	J/mol×K	708.24	Joback Method
cpg	529.04	J/mol×K	742.72	Joback Method
cpg	542.27	J/mol×K	777.19	Joback Method

cpg	554.69	J/mol×K	811.67	Joback Method
dvisc	0.0027727	Pa×s	321.41	Joback Method
dvisc	0.0013027	Pa×s	368.64	Joback Method
dvisc	0.0007266	Pa×s	415.88	Joback Method
dvisc	0.0004566	Pa×s	463.11	Joback Method
dvisc	0.0003126	Pa×s	510.34	Joback Method
dvisc	0.0002283	Pa×s	557.58	Joback Method
dvisc	0.0001751	Pa×s	604.81	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R228907&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume