6-Methyl-6-(3-methylphenyl)-2-heptanone

Other names: 2-Heptanone, 6-methyl-6-(3-methylphenyl)
Inchi: InChI=1S/C15H22O/c1-12-7-5-9-14(11-12)15(3,4)10-6-8-13(2)16/h5,7,9,11H,6,8,10H2,1-
InchiKey: AUFVFYVDFCCOQQ-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC(=O)CCCC(C)(C)c1cccc(C)c1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	52.12	kJ/mol	Joback Method
hf	-249.20	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.032		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	624.90	K	Joback Method
tc	836.01	K	Joback Method
tf	350.10	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.24	J/mol×K	624.90	Joback Method
cpg	539.02	J/mol×K	660.08	Joback Method
cpg	555.69	J/mol×K	695.27	Joback Method
cpg	571.29	J/mol×K	730.45	Joback Method
cpg	585.90	J/mol×K	765.64	Joback Method
cpg	599.56	J/mol×K	800.82	Joback Method
cpg	612.35	J/mol×K	836.01	Joback Method

dvisc	0.0023446	Pa×s	350.10	Joback Method
dvisc	0.0011364	Pa×s	395.90	Joback Method
dvisc	0.0006401	Pa×s	441.70	Joback Method
dvisc	0.0004016	Pa×s	487.50	Joback Method
dvisc	0.0002730	Pa×s	533.30	Joback Method
dvisc	0.0001972	Pa×s	579.10	Joback Method
dvisc	0.0001494	Pa×s	624.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200058&Units=SI

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