2-Heptenoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H18O2/c1-3-4-5-6-10-14(15)16-13-9-7-8-12(2)11-13/h6-11H,3-5H2,1-2H3/
InchiKey: AFDOMHJVYWVYGL-UXBLZVDNSA-N
Formula: C14H18O2
SMILES: CCCCC=CC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	16.08	kJ/mol	Joback Method
hf	-234.81	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.647		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
tb	631.83	K	Joback Method
tc	840.79	K	Joback Method
tf	353.56	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.86	J/mol×K	631.83	Joback Method
cpg	542.23	J/mol×K	805.96	Joback Method
cpg	530.04	J/mol×K	771.13	Joback Method
cpg	517.05	J/mol×K	736.31	Joback Method
cpg	503.21	J/mol×K	701.48	Joback Method
cpg	488.49	J/mol×K	666.66	Joback Method
cpg	553.65	J/mol×K	840.79	Joback Method
dvisc	0.0001284	Pa×s	631.83	Joback Method

dvisc	0.0001641	Pa×s	585.45	Joback Method
dvisc	0.0002187	Pa×s	539.07	Joback Method
dvisc	0.0003077	Pa×s	492.69	Joback Method
dvisc	0.0004647	Pa×s	446.32	Joback Method
dvisc	0.0007724	Pa×s	399.94	Joback Method
dvisc	0.0014668	Pa×s	353.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406905&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

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

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