8-Phenyloctanoic acid

Inchi: InChI=1S/C14H20O2/c15-14(16)12-8-3-1-2-5-9-13-10-6-4-7-11-13/h4,6-7,10-11H,1-3,5,8
InchiKey: VZECIAZMSHBQOC-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: O=C(O)CCCCCCCc1ccccc1
Mol. weight [g/mol]: 220.31
CAS: 26547-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-86.33	kJ/mol	Joback Method
hf	-360.57	kJ/mol	Joback Method
hfus	31.74	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.654		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	692.45	K	Joback Method
tc	883.91	K	Joback Method
tf	384.71	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.00	J/mol×K	692.45	Joback Method
cpg	541.67	J/mol×K	724.36	Joback Method
cpg	554.55	J/mol×K	756.27	Joback Method
cpg	566.68	J/mol×K	788.18	Joback Method
cpg	578.10	J/mol×K	820.09	Joback Method
cpg	588.83	J/mol×K	852.00	Joback Method
cpg	598.93	J/mol×K	883.91	Joback Method
dvisc	0.0031049	Pa×s	384.71	Joback Method
dvisc	0.0010239	Pa×s	436.00	Joback Method

dvisc	0.0004265	Pa×s	487.29	Joback Method
dvisc	0.0002099	Pa×s	538.58	Joback Method
dvisc	0.0001168	Pa×s	589.87	Joback Method
dvisc	0.0000714	Pa×s	641.16	Joback Method
dvisc	0.0000470	Pa×s	692.45	Joback Method

Sources

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=C26547513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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