7-Phenylheptanoic acid

Inchi: InChI=1S/C13H18O2/c14-13(15)11-7-2-1-4-8-12-9-5-3-6-10-12/h3,5-6,9-10H,1-2,4,7-8,1
InchiKey: ZVSXKFNTWOIGJI-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: O=C(O)CCCCCCc1ccccc1
Mol. weight [g/mol]: 206.28
CAS: 40228-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-94.75	kJ/mol	Joback Method
hf	-339.93	kJ/mol	Joback Method
hfus	29.15	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.264		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2470.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
tb	669.57	K	Joback Method
tc	862.71	K	Joback Method
tf	373.44	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.81	J/mol×K	669.57	Joback Method
cpg	488.99	J/mol×K	701.76	Joback Method
cpg	501.40	J/mol×K	733.95	Joback Method
cpg	513.08	J/mol×K	766.14	Joback Method
cpg	524.07	J/mol×K	798.33	Joback Method
cpg	534.39	J/mol×K	830.52	Joback Method
cpg	544.09	J/mol×K	862.71	Joback Method

dvisc	0.0036643	Pa×s	373.44	Joback Method
dvisc	0.0012141	Pa×s	422.79	Joback Method
dvisc	0.0005068	Pa×s	472.15	Joback Method
dvisc	0.0002496	Pa×s	521.50	Joback Method
dvisc	0.0001389	Pa×s	570.86	Joback Method
dvisc	0.0000849	Pa×s	620.21	Joback Method
dvisc	0.0000558	Pa×s	669.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40228908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids:	https://www.doi.org/10.1021/je060078g
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume