6-Benzoylhexanoic acid

Other names: Benzeneheptanoic acid, «zeta»-oxo-
Inchi: InChI=1S/C13H16O3/c14-12(11-7-3-1-4-8-11)9-5-2-6-10-13(15)16/h1,3-4,7-8H,2,5-6,9-1
InchiKey: DOQWHEUDAHLEPT-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: O=C(O)CCCCCC(=O)c1ccccc1
Mol. weight [g/mol]: 220.26
CAS: 7472-43-7

Physical Properties

Property code	Value	Unit	Source
gf	-223.67	kJ/mol	Joback Method
hf	-452.51	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.904		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	723.44	K	Joback Method
tc	923.39	K	Joback Method
tf	423.37	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.90	J/mol×K	723.44	Joback Method
cpg	542.73	J/mol×K	890.06	Joback Method
cpg	533.75	J/mol×K	856.74	Joback Method
cpg	524.10	J/mol×K	823.41	Joback Method
cpg	513.77	J/mol×K	790.09	Joback Method
cpg	502.72	J/mol×K	756.76	Joback Method
cpg	551.10	J/mol×K	923.39	Joback Method
dvisc	0.0000486	Pa×s	723.44	Joback Method

dvisc	0.0000716	Pa×s	673.43	Joback Method
dvisc	0.0001123	Pa×s	623.42	Joback Method
dvisc	0.0001906	Pa×s	573.40	Joback Method
dvisc	0.0003579	Pa×s	523.39	Joback Method
dvisc	0.0007676	Pa×s	473.38	Joback Method
dvisc	0.0019714	Pa×s	423.37	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=C7472437&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume