

8-Benzoyloctanoic acid

Inchi:	InChI=1S/C15H20O3/c16-14(13-9-5-4-6-10-13)11-7-2-1-3-8-12-15(17)18/h4-6,9-10H,1-3
InchiKey:	BFUPULAAJVYXRI-UHFFFAOYSA-N
Formula:	C15H20O3
SMILES:	O=C(O)CCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	248.32
CAS:	16269-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-206.83	kJ/mol	Joback Method
hf	-493.79	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.685		Crippen Method
mvol	207.460	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	769.20	K	Joback Method
tc	966.53	K	Joback Method
tf	445.91	K	Joback Method
vc	0.798	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.72	J/mol×K	769.20	Joback Method
cpg	610.44	J/mol×K	802.09	Joback Method
cpg	622.35	J/mol×K	834.98	Joback Method
cpg	633.51	J/mol×K	867.86	Joback Method
cpg	643.93	J/mol×K	900.75	Joback Method
cpg	653.66	J/mol×K	933.64	Joback Method
cpg	662.75	J/mol×K	966.53	Joback Method
dvisc	0.0014501	Paxs	445.91	Joback Method
dvisc	0.0005556	Paxs	499.79	Joback Method

dvisc	0.0002566	Paxs	553.67	Joback Method
dvisc	0.0001359	Paxs	607.55	Joback Method
dvisc	0.0000798	Paxs	661.44	Joback Method
dvisc	0.0000508	Paxs	715.32	Joback Method
dvisc	0.0000344	Paxs	769.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C16269059&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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