

Benzenepentanoic acid, «delta»-oxo-

Other names:	4-Benzoylbutyric acid
Inchi:	InChI=1S/C11H12O3/c12-10(7-4-8-11(13)14)9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,13,14)
InchiKey:	SHKWSBAVRQZYLE-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	O=C(O)CCCC(=O)c1ccccc1
Mol. weight [g/mol]:	192.21
CAS:	1501-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-240.51	kJ/mol	Joback Method
hf	-411.23	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.124		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	677.68	K	Joback Method
tc	882.13	K	Joback Method
tf	400.83	K	Joback Method
vc	0.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.98	J/mol×K	677.68	Joback Method
cpg	399.69	J/mol×K	711.76	Joback Method
cpg	409.68	J/mol×K	745.83	Joback Method
cpg	419.00	J/mol×K	779.91	Joback Method
cpg	427.66	J/mol×K	813.98	Joback Method
cpg	435.72	J/mol×K	848.06	Joback Method
cpg	443.19	J/mol×K	882.13	Joback Method
dvisc	0.0026452	Paxs	400.83	Joback Method

dvisc	0.0010489	Paxs	446.97	Joback Method
dvisc	0.0004945	Paxs	493.11	Joback Method
dvisc	0.0002652	Paxs	539.25	Joback Method
dvisc	0.0001569	Paxs	585.40	Joback Method
dvisc	0.0001002	Paxs	631.54	Joback Method
dvisc	0.0000680	Paxs	677.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501059&Units=SI
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

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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