Methyl 4-benzoylbutyrate

Other names: Benzenepentanoic acid, «delta»-oxo-, methyl ester
Inchi: InChI=1S/C12H14O3/c1-15-12(14)9-5-8-11(13)10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3
InchiKey: GRIWFUFDJOESIC-UHFFFAOYSA-N
Formula: C12H14O3
SMILES: COC(=O)CCCC(=O)c1ccccc1
Mol. weight [g/mol]: 206.24
CAS: 1501-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-200.27	kJ/mol	Joback Method
hf	-411.86	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.213		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	630.80	K	Joback Method
tc	844.08	K	Joback Method
tf	373.51	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.34	J/mol×K	630.80	Joback Method
cpg	472.88	J/mol×K	808.53	Joback Method
cpg	462.42	J/mol×K	772.99	Joback Method
cpg	451.15	J/mol×K	737.44	Joback Method
cpg	439.07	J/mol×K	701.89	Joback Method
cpg	426.14	J/mol×K	666.35	Joback Method
cpg	482.56	J/mol×K	844.08	Joback Method
dvisc	0.0001911	Pa×s	630.80	Joback Method

dvisc	0.0002433	Pa×s	587.92	Joback Method
dvisc	0.0003218	Pa×s	545.04	Joback Method
dvisc	0.0004464	Pa×s	502.15	Joback Method
dvisc	0.0006581	Pa×s	459.27	Joback Method
dvisc	0.0010512	Pa×s	416.39	Joback Method
dvisc	0.0018695	Pa×s	373.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.00 ± 1.00	K	0.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1501048&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume