

Benzenepentanoic acid, methyl ester

Other names:	Valeric acid, 5-phenyl-, methyl ester Methyl 5-phenylvalerate
Inchi:	InChI=1S/C12H16O2/c1-14-12(13)10-6-5-9-11-7-3-2-4-8-11/h2-4,7-8H,5-6,9-10H2,1H3
InchiKey:	BNNWLDUOVGYRLY-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	COC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	20620-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-71.35	kJ/mol	Joback Method
hf	-299.28	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.572		Crippen Method
mvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	576.93	K	Joback Method
tc	782.93	K	Joback Method
tf	323.58	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/molxK	576.93	Joback Method
cpg	461.69	J/molxK	748.60	Joback Method
cpg	449.76	J/molxK	714.26	Joback Method
cpg	437.06	J/molxK	679.93	Joback Method
cpg	423.55	J/molxK	645.60	Joback Method
cpg	409.22	J/molxK	611.26	Joback Method
cpg	472.86	J/molxK	782.93	Joback Method

dvisc	0.0001842	Paxs	576.93	Joback Method
dvisc	0.0002371	Paxs	534.70	Joback Method
dvisc	0.0003185	Paxs	492.48	Joback Method
dvisc	0.0004524	Paxs	450.25	Joback Method
dvisc	0.0006908	Paxs	408.03	Joback Method
dvisc	0.0011633	Paxs	365.81	Joback Method
dvisc	0.0022442	Paxs	323.58	Joback Method

Sources

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=C20620591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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