5-Phenylvaleric acid, butyl ester

Inchi: InChI=1S/C15H22O2/c1-2-3-13-17-15(16)12-8-7-11-14-9-5-4-6-10-14/h4-6,9-10H,2-3,7-8
InchiKey: JCPKEAYFCLXQJT-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-46.09	kJ/mol	Joback Method
hf	-361.20	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.743		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	645.57	K	Joback Method
tc	843.08	K	Joback Method
tf	357.39	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.39	J/mol×K	645.57	Joback Method
cpg	563.17	J/mol×K	678.49	Joback Method
cpg	579.02	J/mol×K	711.41	Joback Method
cpg	593.96	J/mol×K	744.32	Joback Method
cpg	608.02	J/mol×K	777.24	Joback Method
cpg	621.23	J/mol×K	810.16	Joback Method
cpg	633.62	J/mol×K	843.08	Joback Method
dvisc	0.0019370	Pa×s	357.39	Joback Method

dvisc	0.0009578	Pa×s	405.42	Joback Method
dvisc	0.0005498	Pa×s	453.45	Joback Method
dvisc	0.0003510	Pa×s	501.48	Joback Method
dvisc	0.0002424	Pa×s	549.51	Joback Method
dvisc	0.0001776	Pa×s	597.54	Joback Method
dvisc	0.0001364	Pa×s	645.57	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=U406072&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume