5-Phenylvaleric acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C24H24O3/c25-24(14-8-7-11-20-9-3-1-4-10-20)27-23-17-15-22(16-18-23)26-1
InchiKey: FLPKMKUBKOGWHP-UHFFFAOYSA-N
Formula: C24H24O3
SMILES: O=C(CCCCc1ccccc1)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 360.45

Physical Properties

Property code	Value	Unit	Source
gf	139.88	kJ/mol	Joback Method
hf	-217.59	kJ/mol	Joback Method
hfus	43.62	kJ/mol	Joback Method
hvap	88.07	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.584		Crippen Method
mcvol	291.050	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2963.00		NIST Webbook
rinpol	2963.00		NIST Webbook
tb	932.25	K	Joback Method
tc	1171.23	K	Joback Method
tf	546.41	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.13	J/mol×K	932.25	Joback Method
cpg	915.63	J/mol×K	972.08	Joback Method
cpg	928.66	J/mol×K	1011.91	Joback Method
cpg	940.31	J/mol×K	1051.74	Joback Method
cpg	950.64	J/mol×K	1091.57	Joback Method
cpg	959.74	J/mol×K	1131.40	Joback Method
cpg	967.68	J/mol×K	1171.23	Joback Method
dvisc	0.0003632	Pa×s	546.41	Joback Method

dvisc	0.0001995	Pa×s	610.72	Joback Method
dvisc	0.0001228	Pa×s	675.02	Joback Method
dvisc	0.0000823	Pa×s	739.33	Joback Method
dvisc	0.0000588	Pa×s	803.64	Joback Method
dvisc	0.0000441	Pa×s	867.94	Joback Method
dvisc	0.0000345	Pa×s	932.25	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=U406902&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