

Valeric acid, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C18H20O3/c1-2-3-9-18(19)21-17-12-10-16(11-13-17)20-14-15-7-5-4-6-8-15/h
InchiKey:	IGPTVJONPUIQKC-UHFFFAOYSA-N
Formula:	C18H20O3
SMILES:	CCCCC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	284.35

Physical Properties

Property code	Value	Unit	Source
gf	-23.05	kJ/mol	Joback Method
hf	-330.28	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	72.44	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.361		Crippen Method
mcvol	230.270	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpola	2295.00		NIST Webbook
tb	768.29	K	Joback Method
tc	991.36	K	Joback Method
tf	452.37	K	Joback Method
vc	0.870	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.48	J/molxK	768.29	Joback Method
cpg	721.48	J/molxK	954.18	Joback Method
cpg	710.19	J/molxK	917.00	Joback Method
cpg	697.78	J/molxK	879.82	Joback Method
cpg	684.22	J/molxK	842.65	Joback Method
cpg	669.46	J/molxK	805.47	Joback Method
cpg	731.68	J/molxK	991.36	Joback Method
dvisc	0.0000747	Paxs	768.29	Joback Method
dvisc	0.0000950	Paxs	715.64	Joback Method

dvisc	0.0001255	Paxs	662.98	Joback Method
dvisc	0.0001741	Paxs	610.33	Joback Method
dvisc	0.0002567	Paxs	557.68	Joback Method
dvisc	0.0004105	Paxs	505.02	Joback Method
dvisc	0.0007322	Paxs	452.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307991&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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