

5-Phenylvaleric acid, 3-methylphenyl ester

Inchi:	InChI=1S/C18H20O2/c1-15-8-7-12-17(14-15)20-18(19)13-6-5-11-16-9-3-2-4-10-16/h2-4,
InchiKey:	XITFYZFKGYNNNR-UHFFFAOYSA-N
Formula:	C18H20O2
SMILES:	<chem>Cc1cccc(OC(=O)CCCCc2ccccc2)c1</chem>
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	81.95	kJ/mol	Joback Method
hf	-198.06	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.313		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	745.87	K	Joback Method
tc	971.40	K	Joback Method
tf	430.14	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.86	J/molxK	745.87	Joback Method
cpg	642.38	J/molxK	783.46	Joback Method
cpg	657.68	J/molxK	821.05	Joback Method
cpg	671.82	J/molxK	858.63	Joback Method
cpg	684.83	J/molxK	896.22	Joback Method
cpg	696.78	J/molxK	933.81	Joback Method
cpg	707.72	J/molxK	971.40	Joback Method
dvisc	0.0010197	Paxs	430.14	Joback Method

dvisc	0.0005566	Paxs	482.76	Joback Method
dvisc	0.0003422	Paxs	535.38	Joback Method
dvisc	0.0002295	Paxs	588.00	Joback Method
dvisc	0.0001644	Paxs	640.63	Joback Method
dvisc	0.0001239	Paxs	693.25	Joback Method
dvisc	0.0000971	Paxs	745.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406899&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
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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