

5-Phenylvaleric acid, heptyl ester

Inchi:	InChI=1S/C18H28O2/c1-2-3-4-5-11-16-20-18(19)15-10-9-14-17-12-7-6-8-13-17/h6-8,12-
InchiKey:	OSNYCQLSEGDSMO-UHFFFAOYSA-N
Formula:	C18H28O2
SMILES:	CCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	276.41

Physical Properties

Property code	Value	Unit	Source
gf	-20.83	kJ/mol	Joback Method
hf	-423.12	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.913		Crippen Method
mvol	248.160	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	714.21	K	Joback Method
tc	906.19	K	Joback Method
tf	391.20	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.91	J/molxK	714.21	Joback Method
cpg	728.69	J/molxK	746.21	Joback Method
cpg	745.47	J/molxK	778.20	Joback Method
cpg	761.28	J/molxK	810.20	Joback Method
cpg	776.16	J/molxK	842.20	Joback Method
cpg	790.14	J/molxK	874.20	Joback Method
cpg	803.25	J/molxK	906.19	Joback Method
dvisc	0.0015490	Paxs	391.20	Joback Method

dvisc	0.0007359	Paxs	445.03	Joback Method
dvisc	0.0004105	Paxs	498.87	Joback Method
dvisc	0.0002566	Paxs	552.70	Joback Method
dvisc	0.0001743	Paxs	606.54	Joback Method
dvisc	0.0001261	Paxs	660.38	Joback Method
dvisc	0.0000958	Paxs	714.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406076&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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