

5-Phenylvaleric acid, hexadecyl ester

Inchi:	InChI=1S/C27H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-25-29-27(28)24-19-18-23-26
InchiKey:	LJROKOFJSTZXQD-UHFFFAOYSA-N
Formula:	C27H46O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	402.65

Physical Properties

Property code	Value	Unit	Source
gf	54.95	kJ/mol	Joback Method
hf	-608.88	kJ/mol	Joback Method
hfus	62.51	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	8.424		Crippen Method
mvol	374.970	ml/mol	McGowan Method
pc	848.50	kPa	Joback Method
rinpol	3024.00		NIST Webbook
rinpol	3024.00		NIST Webbook
tb	920.13	K	Joback Method
tc	1126.50	K	Joback Method
tf	492.63	K	Joback Method
vc	1.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.14	J/molxK	920.13	Joback Method
cpg	1344.97	J/molxK	1092.10	Joback Method
cpg	1329.63	J/molxK	1057.71	Joback Method
cpg	1313.14	J/molxK	1023.31	Joback Method
cpg	1295.44	J/molxK	988.92	Joback Method
cpg	1276.46	J/molxK	954.52	Joback Method
cpg	1359.23	J/molxK	1126.50	Joback Method
dvisc	0.0000275	Paxs	920.13	Joback Method

dvisc	0.0000370	Paxs	848.88	Joback Method
dvisc	0.0000526	Paxs	777.63	Joback Method
dvisc	0.0000802	Paxs	706.38	Joback Method
dvisc	0.0001345	Paxs	635.13	Joback Method
dvisc	0.0002570	Paxs	563.88	Joback Method
dvisc	0.0005922	Paxs	492.63	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=U406085&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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