

5-Phenylvaleric acid, pentadecyl ester

Inchi:	InChI=1S/C26H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-24-28-26(27)23-18-17-22-25-20
InchiKey:	XDIUOTCIPHNLOB-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	388.63

Physical Properties

Property code	Value	Unit	Source
gf	46.53	kJ/mol	Joback Method
hf	-588.24	kJ/mol	Joback Method
hfus	59.92	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.034		Crippen Method
mvol	360.880	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpol	2919.00		NIST Webbook
rinpol	2919.00		NIST Webbook
tb	897.25	K	Joback Method
tc	1098.93	K	Joback Method
tf	481.36	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.71	J/molxK	897.25	Joback Method
cpg	1212.65	J/molxK	930.86	Joback Method
cpg	1231.30	J/molxK	964.48	Joback Method
cpg	1248.73	J/molxK	998.09	Joback Method
cpg	1265.00	J/molxK	1031.70	Joback Method
cpg	1280.17	J/molxK	1065.31	Joback Method
cpg	1294.30	J/molxK	1098.93	Joback Method
dvisc	0.0006695	Paxs	481.36	Joback Method

dvisc	0.0002930	Paxs	550.67	Joback Method
dvisc	0.0001542	Paxs	619.99	Joback Method
dvisc	0.0000924	Paxs	689.30	Joback Method
dvisc	0.0000608	Paxs	758.62	Joback Method
dvisc	0.0000429	Paxs	827.93	Joback Method
dvisc	0.0000319	Paxs	897.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406084&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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