

5-Phenylvaleric acid, octadecyl ester

Inchi:	InChI=1S/C29H50O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-27-31-29(30)26-21-20
InchiKey:	DVLVBBBQVOVUQF-UHFFFAOYSA-N
Formula:	C29H50O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	430.71

Physical Properties

Property code	Value	Unit	Source
gf	71.79	kJ/mol	Joback Method
hf	-650.16	kJ/mol	Joback Method
hfus	67.69	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-9.93		Crippen Method
logp	9.204		Crippen Method
mvol	403.150	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	3237.00		NIST Webbook
rinpol	3237.00		NIST Webbook
tb	965.89	K	Joback Method
tc	1184.68	K	Joback Method
tf	515.17	K	Joback Method
vc	1.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.52	J/molxK	965.89	Joback Method
cpg	1476.64	J/molxK	1148.22	Joback Method
cpg	1460.89	J/molxK	1111.75	Joback Method
cpg	1443.89	J/molxK	1075.29	Joback Method
cpg	1425.55	J/molxK	1038.82	Joback Method
cpg	1405.79	J/molxK	1002.36	Joback Method
cpg	1491.24	J/molxK	1184.68	Joback Method
dvisc	0.0000203	Paxs	965.89	Joback Method

dvisc	0.0000274	Paxs	890.77	Joback Method
dvisc	0.0000392	Paxs	815.65	Joback Method
dvisc	0.0000601	Paxs	740.53	Joback Method
dvisc	0.0001016	Paxs	665.41	Joback Method
dvisc	0.0001962	Paxs	590.29	Joback Method
dvisc	0.0004593	Paxs	515.17	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=U406087&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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