

5-Phenylvaleric acid, tetradecyl ester

Inchi:	InChI=1S/C25H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-18-23-27-25(26)22-17-16-21-24-19-14
InchiKey:	USGFNSBZBPBSML-UHFFFAOYSA-N
Formula:	C25H42O2
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	374.60

Physical Properties

Property code	Value	Unit	Source
gf	38.11	kJ/mol	Joback Method
hf	-567.60	kJ/mol	Joback Method
hfus	57.33	kJ/mol	Joback Method
hvap	82.68	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.644		Crippen Method
mvol	346.790	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	2819.00		NIST Webbook
rinpol	2819.00		NIST Webbook
tb	874.37	K	Joback Method
tc	1072.27	K	Joback Method
tf	470.09	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.86	J/molxK	874.37	Joback Method
cpg	1149.45	J/molxK	907.35	Joback Method
cpg	1167.82	J/molxK	940.34	Joback Method
cpg	1185.01	J/molxK	973.32	Joback Method
cpg	1201.09	J/molxK	1006.30	Joback Method
cpg	1216.10	J/molxK	1039.29	Joback Method
cpg	1230.10	J/molxK	1072.27	Joback Method
dvisc	0.0007543	Paxs	470.09	Joback Method

dvisc	0.0003330	Paxs	537.47	Joback Method
dvisc	0.0001764	Paxs	604.85	Joback Method
dvisc	0.0001061	Paxs	672.23	Joback Method
dvisc	0.0000700	Paxs	739.61	Joback Method
dvisc	0.0000495	Paxs	806.99	Joback Method
dvisc	0.0000370	Paxs	874.37	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=U406083&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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