

5-Phenylvaleric acid, tridecyl ester

Inchi:	InChI=1S/C24H40O2/c1-2-3-4-5-6-7-8-9-10-11-17-22-26-24(25)21-16-15-20-23-18-13-12
InchiKey:	FVJLOOXMSXBFRL-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
gf	29.69	kJ/mol	Joback Method
hf	-546.96	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.254		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	851.49	K	Joback Method
tc	1046.47	K	Joback Method
tf	458.82	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.64	J/molxK	851.49	Joback Method
cpg	1152.77	J/molxK	1013.97	Joback Method
cpg	1137.91	J/molxK	981.47	Joback Method
cpg	1122.01	J/molxK	948.98	Joback Method
cpg	1105.03	J/molxK	916.48	Joback Method
cpg	1086.92	J/molxK	883.99	Joback Method
cpg	1166.66	J/molxK	1046.47	Joback Method
dvisc	0.0000427	Paxs	851.49	Joback Method

dvisc	0.0000571	Paxs	786.04	Joback Method
dvisc	0.0000805	Paxs	720.60	Joback Method
dvisc	0.0001216	Paxs	655.15	Joback Method
dvisc	0.0002011	Paxs	589.71	Joback Method
dvisc	0.0003773	Paxs	524.26	Joback Method
dvisc	0.0008470	Paxs	458.82	Joback Method

Sources

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=U406082&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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