Butyric acid, 2-phenyl-, pentadecyl ester

Inchi: InChI=1S/C25H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-22-27-25(26)24(4-2)23-20-17
InchiKey: ZBYDLQCOSGASBR-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
gf	35.67	kJ/mol	Joback Method
hf	-572.88	kJ/mol	Joback Method
hfus	53.81	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.815		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	956.73	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	873.93	K	Joback Method
tc	1072.51	K	Joback Method
tf	455.09	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.30	J/mol×K	873.93	Joback Method
cpg	1149.94	J/mol×K	907.03	Joback Method
cpg	1168.34	J/mol×K	940.12	Joback Method
cpg	1185.55	J/mol×K	973.22	Joback Method
cpg	1201.62	J/mol×K	1006.32	Joback Method
cpg	1216.61	J/mol×K	1039.42	Joback Method
cpg	1230.57	J/mol×K	1072.51	Joback Method
dvisc	0.0008889	Pa×s	455.09	Joback Method

dvisc	0.0003588	Pa×s	524.90	Joback Method
dvisc	0.0001792	Pa×s	594.70	Joback Method
dvisc	0.0001036	Pa×s	664.51	Joback Method
dvisc	0.0000664	Pa×s	734.32	Joback Method
dvisc	0.0000460	Pa×s	804.12	Joback Method
dvisc	0.0000338	Pa×s	873.93	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=U406026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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