Butyric acid, 2-phenyl-, heptadecyl ester

Inchi: InChI=1S/C27H46O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-21-24-29-27(28)26(4-2)25
InchiKey: NPIDHRRXJVVTOS-UHFFFAOYSA-N
Formula: C27H46O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 402.65

Physical Properties

Property code	Value	Unit	Source
gf	52.51	kJ/mol	Joback Method
hf	-614.16	kJ/mol	Joback Method
hfus	58.99	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	8.595		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
pc	852.47	kPa	Joback Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook
tb	919.69	K	Joback Method
tc	1126.02	K	Joback Method
tf	477.63	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.54	J/mol×K	919.69	Joback Method
cpg	1276.83	J/mol×K	954.08	Joback Method
cpg	1295.76	J/mol×K	988.47	Joback Method
cpg	1313.40	J/mol×K	1022.85	Joback Method
cpg	1329.82	J/mol×K	1057.24	Joback Method
cpg	1345.08	J/mol×K	1091.63	Joback Method
cpg	1359.25	J/mol×K	1126.02	Joback Method
dvisc	0.0006899	Pa×s	477.63	Joback Method

dvisc	0.0002746	Pa×s	551.31	Joback Method
dvisc	0.0001358	Pa×s	624.98	Joback Method
dvisc	0.0000779	Pa×s	698.66	Joback Method
dvisc	0.0000497	Pa×s	772.34	Joback Method
dvisc	0.0000343	Pa×s	846.01	Joback Method
dvisc	0.0000251	Pa×s	919.69	Joback Method

Sources

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=U406028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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