Butyric acid, 4-phenyl-, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C16H24O2/c1-13(2)12-14(3)18-16(17)11-7-10-15-8-5-4-6-9-15/h4-6,8-9,13-14
InchiKey: UBZQGOAHCCGUHQ-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CC(C)CC(C)OC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-42.55	kJ/mol	Joback Method
hf	-392.40	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.987		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	667.57	K	Joback Method
tc	869.62	K	Joback Method
tf	338.66	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.91	J/mol×K	667.57	Joback Method
cpg	618.73	J/mol×K	701.25	Joback Method
cpg	635.52	J/mol×K	734.92	Joback Method
cpg	651.29	J/mol×K	768.60	Joback Method
cpg	666.08	J/mol×K	802.27	Joback Method
cpg	679.92	J/mol×K	835.95	Joback Method
cpg	692.85	J/mol×K	869.62	Joback Method
dvisc	0.0029518	Pa×s	338.66	Joback Method

dvisc	0.0011486	Pa×s	393.48	Joback Method
dvisc	0.0005630	Pa×s	448.30	Joback Method
dvisc	0.0003224	Pa×s	503.12	Joback Method
dvisc	0.0002059	Pa×s	557.93	Joback Method
dvisc	0.0001426	Pa×s	612.75	Joback Method
dvisc	0.0001048	Pa×s	667.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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