Butyric acid, 4-phenyl-, dodecyl ester

Inchi: InChI=1S/C22H36O2/c1-2-3-4-5-6-7-8-9-10-14-20-24-22(23)19-15-18-21-16-12-11-13-17
InchiKey: YJLODNCCNAKLHX-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCCCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	12.85	kJ/mol	Joback Method
hf	-505.68	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.473		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	805.73	K	Joback Method
tc	997.16	K	Joback Method
tf	436.28	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.31	J/mol×K	805.73	Joback Method
cpg	1028.49	J/mol×K	965.25	Joback Method
cpg	1013.89	J/mol×K	933.35	Joback Method
cpg	998.31	J/mol×K	901.44	Joback Method
cpg	981.72	J/mol×K	869.54	Joback Method
cpg	964.06	J/mol×K	837.63	Joback Method
cpg	1042.15	J/mol×K	997.16	Joback Method
dvisc	0.0000566	Pa×s	805.73	Joback Method

dvisc	0.0000753	Pa×s	744.15	Joback Method
dvisc	0.0001056	Pa×s	682.58	Joback Method
dvisc	0.0001582	Pa×s	621.00	Joback Method
dvisc	0.0002591	Pa×s	559.43	Joback Method
dvisc	0.0004794	Pa×s	497.85	Joback Method
dvisc	0.0010554	Pa×s	436.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406182&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

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