Butyric acid, 2-phenyl-, dodecyl ester

Inchi: InChI=1S/C22H36O2/c1-3-5-6-7-8-9-10-11-12-16-19-24-22(23)21(4-2)20-17-14-13-15-18
InchiKey: NXLJLCOMNSVHIZ-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	10.41	kJ/mol	Joback Method
hf	-510.96	kJ/mol	Joback Method
hfus	46.04	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.644		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	805.29	K	Joback Method
tc	998.37	K	Joback Method
tf	421.28	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.79	J/mol×K	805.29	Joback Method
cpg	1029.50	J/mol×K	966.19	Joback Method
cpg	1014.85	J/mol×K	934.01	Joback Method
cpg	999.20	J/mol×K	901.83	Joback Method
cpg	982.49	J/mol×K	869.65	Joback Method
cpg	964.71	J/mol×K	837.47	Joback Method
cpg	1043.19	J/mol×K	998.37	Joback Method
dvisc	0.0000520	Pa×s	805.29	Joback Method

dvisc	0.0000703	Pa×s	741.29	Joback Method
dvisc	0.0001008	Pa×s	677.29	Joback Method
dvisc	0.0001557	Pa×s	613.28	Joback Method
dvisc	0.0002661	Pa×s	549.28	Joback Method
dvisc	0.0005239	Pa×s	485.28	Joback Method
dvisc	0.0012673	Pa×s	421.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406023&Units=SI

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