Butyric acid, 2-phenyl-, dec-2-yl ester

Inchi: InChI=1S/C20H32O2/c1-4-6-7-8-9-11-14-17(3)22-20(21)19(5-2)18-15-12-10-13-16-18/h1
InchiKey: YCJYBWZDPUJMEG-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCC(C)OC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	-8.87	kJ/mol	Joback Method
hf	-474.96	kJ/mol	Joback Method
hfus	37.34	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.863		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2007.00		NIST Webbook
tb	759.09	K	Joback Method
tc	954.28	K	Joback Method
tf	383.74	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.19	J/mol×K	759.09	Joback Method
cpg	845.94	J/mol×K	791.62	Joback Method
cpg	863.57	J/mol×K	824.15	Joback Method
cpg	880.12	J/mol×K	856.68	Joback Method
cpg	895.64	J/mol×K	889.21	Joback Method
cpg	910.15	J/mol×K	921.75	Joback Method
cpg	923.71	J/mol×K	954.28	Joback Method
dvisc	0.0019655	Pa×s	383.74	Joback Method
dvisc	0.0007409	Pa×s	446.30	Joback Method

dvisc	0.0003550	Pa×s	508.86	Joback Method
dvisc	0.0001998	Pa×s	571.41	Joback Method
dvisc	0.0001260	Pa×s	633.97	Joback Method
dvisc	0.0000863	Pa×s	696.53	Joback Method
dvisc	0.0000629	Pa×s	759.09	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=U406864&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

Latest version available from:
https://www.chemeo.com/cid/87-625-2/Butyric-acid-2-phenyl-dec-2-yl-ester.pdf
Generated by Cheméo on 2024-10-12 07:23:34.462309569 +0000 UTC m=+3298677.099278822.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.