

Butyric acid, 2-phenyl-, tridecyl ester

Inchi:	InChI=1S/C23H38O2/c1-3-5-6-7-8-9-10-11-12-13-17-20-25-23(24)22(4-2)21-18-15-14-16
InchiKey:	JCIUACIYRVMVJG-UHFFFAOYSA-N
Formula:	C23H38O2
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	346.55

Physical Properties

Property code	Value	Unit	Source
gf	18.83	kJ/mol	Joback Method
hf	-531.60	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	7.034		Crippen Method
mvol	318.610	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	828.17	K	Joback Method
tc	1022.35	K	Joback Method
tf	432.55	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.57	J/molxK	828.17	Joback Method
cpg	1091.09	J/molxK	989.99	Joback Method
cpg	1076.33	J/molxK	957.62	Joback Method
cpg	1060.54	J/molxK	925.26	Joback Method
cpg	1043.68	J/molxK	892.90	Joback Method
cpg	1025.71	J/molxK	860.53	Joback Method
cpg	1104.87	J/molxK	1022.35	Joback Method
dvisc	0.0000452	Paxs	828.17	Joback Method

dvisc	0.0000612	Paxs	762.23	Joback Method
dvisc	0.0000880	Paxs	696.30	Joback Method
dvisc	0.0001363	Paxs	630.36	Joback Method
dvisc	0.0002340	Paxs	564.42	Joback Method
dvisc	0.0004634	Paxs	498.49	Joback Method
dvisc	0.0011302	Paxs	432.55	Joback Method

Sources

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=U406024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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