Butyric acid, 4-phenyl-, tridecyl ester

Inchi: InChI=1S/C23H38O2/c1-2-3-4-5-6-7-8-9-10-11-15-21-25-23(24)20-16-19-22-17-13-12-14
InchiKey: SUTKPZUBWYBYIE-UHFFFAOYSA-N
Formula: C23H38O2
SMILES: CCCCCCCCCCCCCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 346.55

Physical Properties

Property code	Value	Unit	Source
gf	21.27	kJ/mol	Joback Method
hf	-526.32	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.864		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	828.61	K	Joback Method
tc	1021.45	K	Joback Method
tf	447.55	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.10	J/mol×K	828.61	Joback Method
cpg	1025.11	J/mol×K	860.75	Joback Method
cpg	1042.98	J/mol×K	892.89	Joback Method
cpg	1059.76	J/mol×K	925.03	Joback Method
cpg	1075.50	J/mol×K	957.17	Joback Method
cpg	1090.23	J/mol×K	989.31	Joback Method
cpg	1104.00	J/mol×K	1021.45	Joback Method
dvisc	0.0009474	Pa×s	447.55	Joback Method

dvisc	0.0004261	Pa×s	511.06	Joback Method
dvisc	0.0002287	Pa×s	574.57	Joback Method
dvisc	0.0001389	Pa×s	638.08	Joback Method
dvisc	0.0000923	Pa×s	701.59	Joback Method
dvisc	0.0000657	Pa×s	765.10	Joback Method
dvisc	0.0000492	Pa×s	828.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406183&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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