

Butyric acid, 4-phenyl-, nonyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H30O2/c1-2-3-4-5-6-7-11-17-21-19(20)16-12-15-18-13-9-8-10-14-18/h8-10

OUVDUDLJCSORPT-UHFFFAOYSA-N

C19H30O2

CCCCCCCCCOC(=O)CCCC1CCCCC1

290.44

Physical Properties

Property code	Value	Unit	Source
gf	-12.41	kJ/mol	Joback Method
hf	-443.76	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.303		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	737.09	K	Joback Method
tc	928.11	K	Joback Method
tf	402.47	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.05	J/mol×K	737.09	Joback Method
cpg	786.09	J/mol×K	768.93	Joback Method
cpg	803.11	J/mol×K	800.76	Joback Method
cpg	819.14	J/mol×K	832.60	Joback Method
cpg	834.22	J/mol×K	864.43	Joback Method
cpg	848.38	J/mol×K	896.27	Joback Method
cpg	861.65	J/mol×K	928.11	Joback Method
dvisc	0.0014187	Pa×s	402.47	Joback Method

dvisc	0.0006659	Pa×s	458.24	Joback Method
dvisc	0.0003683	Pa×s	514.01	Joback Method
dvisc	0.0002288	Pa×s	569.78	Joback Method
dvisc	0.0001547	Pa×s	625.55	Joback Method
dvisc	0.0001115	Pa×s	681.32	Joback Method
dvisc	0.0000845	Pa×s	737.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406179&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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