

Butyric acid, 2-phenyl-, decyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-6.43	kJ/mol	Joback Method
hf	-469.68	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.864		Crippen Method
mvol	276.340	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	759.53	K	Joback Method
tc	952.34	K	Joback Method
tf	398.74	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	759.53	Joback Method
cpg	845.21	J/mol×K	791.66	Joback Method
cpg	862.64	J/mol×K	823.80	Joback Method
cpg	879.02	J/mol×K	855.93	Joback Method
cpg	894.41	J/mol×K	888.07	Joback Method
cpg	908.82	J/mol×K	920.20	Joback Method
cpg	922.31	J/mol×K	952.34	Joback Method
dvisc	0.0015731	Paxs	398.74	Joback Method

dvisc	0.0006621	Paxs	458.87	Joback Method
dvisc	0.0003406	Paxs	519.00	Joback Method
dvisc	0.0002011	Paxs	579.13	Joback Method
dvisc	0.0001311	Paxs	639.27	Joback Method
dvisc	0.0000920	Paxs	699.40	Joback Method
dvisc	0.0000683	Paxs	759.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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