

Butyric acid, 2-phenyl-, hexyl ester

Inchi:	InChI=1S/C16H24O2/c1-3-5-6-10-13-18-16(17)15(4-2)14-11-8-7-9-12-14/h7-9,11-12,15H
InchiKey:	IZZRASDRHNCNSR-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	-40.11	kJ/mol	Joback Method
hf	-387.12	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.304		Crippen Method
mvol	219.980	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
tb	668.01	K	Joback Method
tc	866.60	K	Joback Method
tf	353.66	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.45	J/molxK	668.01	Joback Method
cpg	678.21	J/molxK	833.50	Joback Method
cpg	664.53	J/molxK	800.40	Joback Method
cpg	649.95	J/molxK	767.31	Joback Method
cpg	634.43	J/molxK	734.21	Joback Method
cpg	617.94	J/molxK	701.11	Joback Method
cpg	691.01	J/molxK	866.60	Joback Method
dvisc	0.0001130	Paxs	668.01	Joback Method

dvisc	0.0001506	Paxs	615.62	Joback Method
dvisc	0.0002118	Paxs	563.23	Joback Method
dvisc	0.0003195	Paxs	510.84	Joback Method
dvisc	0.0005293	Paxs	458.44	Joback Method
dvisc	0.0009989	Paxs	406.05	Joback Method
dvisc	0.0022754	Paxs	353.66	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=U406017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h_{vap}:	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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