

Butyric acid, 2-phenyl-, heptyl ester

Inchi:	InChI=1S/C17H26O2/c1-3-5-6-7-11-14-19-17(18)16(4-2)15-12-9-8-10-13-15/h8-10,12-13
InchiKey:	CPAVSVYEWNICIE-UHFFFAOYSA-N
Formula:	C17H26O2
SMILES:	CCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	262.39

Physical Properties

Property code	Value	Unit	Source
gf	-31.69	kJ/mol	Joback Method
hf	-407.76	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.694		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	1831.00		NIST Webbook
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tb	690.89	K	Joback Method
tc	887.37	K	Joback Method
tf	364.93	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.33	J/molxK	690.89	Joback Method
cpg	673.13	J/molxK	723.64	Joback Method
cpg	689.91	J/molxK	756.38	Joback Method
cpg	705.70	J/molxK	789.13	Joback Method
cpg	720.53	J/molxK	821.87	Joback Method
cpg	734.45	J/molxK	854.62	Joback Method
cpg	747.47	J/molxK	887.37	Joback Method
dvisc	0.0020940	Paxs	364.93	Joback Method

dvisc	0.0009088	Paxs	419.26	Joback Method
dvisc	0.0004777	Paxs	473.58	Joback Method
dvisc	0.0002866	Paxs	527.91	Joback Method
dvisc	0.0001892	Paxs	582.24	Joback Method
dvisc	0.0001340	Paxs	636.56	Joback Method
dvisc	0.0001003	Paxs	690.89	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=U406018&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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