

Butyric acid, 2-phenyl-, 8-chlorooctyl ester

Inchi:	InChI=1S/C18H27ClO2/c1-2-17(16-12-8-7-9-13-16)18(20)21-15-11-6-4-3-5-10-14-19/h7-
InchiKey:	IJRVMEJOHOAYMY-UHFFFAOYSA-N
Formula:	C18H27ClO2
SMILES:	CCC(C(=O)OCCCCCCCCCl)c1ccccc1
Mol. weight [g/mol]:	310.86

Physical Properties

Property code	Value	Unit	Source
gf	-35.20	kJ/mol	Joback Method
hf	-444.14	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.303		Crippen Method
mvol	260.400	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	751.20	K	Joback Method
tc	949.94	K	Joback Method
tf	406.12	K	Joback Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.41	J/molxK	751.20	Joback Method
cpg	759.32	J/molxK	784.32	Joback Method
cpg	775.20	J/molxK	817.45	Joback Method
cpg	790.07	J/molxK	850.57	Joback Method
cpg	803.99	J/molxK	883.69	Joback Method
cpg	816.98	J/molxK	916.81	Joback Method
cpg	829.08	J/molxK	949.94	Joback Method
dvisc	0.0015158	Paxs	406.12	Joback Method

dvisc	0.0006817	Paxs	463.63	Joback Method
dvisc	0.0003657	Paxs	521.15	Joback Method
dvisc	0.0002221	Paxs	578.66	Joback Method
dvisc	0.0001476	Paxs	636.17	Joback Method
dvisc	0.0001049	Paxs	693.69	Joback Method
dvisc	0.0000786	Paxs	751.20	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=U406866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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