

Butyric acid, 2-phenyl-, octadecyl ester

Inchi:	InChI=1S/C28H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-25-30-28(29)27(4-2
InchiKey:	LTESNJQASILVDY-UHFFFAOYSA-N
Formula:	C28H48O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	416.68

Physical Properties

Property code	Value	Unit	Source
gf	60.93	kJ/mol	Joback Method
hf	-634.80	kJ/mol	Joback Method
hfus	61.58	kJ/mol	Joback Method
hvap	88.97	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.985		Crippen Method
mvol	389.060	ml/mol	McGowan Method
pc	806.62	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	942.57	K	Joback Method
tc	1154.19	K	Joback Method
tf	488.90	K	Joback Method
vc	1.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.46	J/molxK	942.57	Joback Method
cpg	1410.37	J/molxK	1118.92	Joback Method
cpg	1394.94	J/molxK	1083.65	Joback Method
cpg	1378.31	J/molxK	1048.38	Joback Method
cpg	1360.40	J/molxK	1013.11	Joback Method
cpg	1341.15	J/molxK	977.84	Joback Method
cpg	1424.66	J/molxK	1154.19	Joback Method
dvisc	0.0000216	Paxs	942.57	Joback Method

dvisc	0.0000295	Paxs	866.96	Joback Method
dvisc	0.0000429	Paxs	791.35	Joback Method
dvisc	0.0000674	Paxs	715.73	Joback Method
dvisc	0.0001178	Paxs	640.12	Joback Method
dvisc	0.0002393	Paxs	564.51	Joback Method
dvisc	0.0006052	Paxs	488.90	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=U406029&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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