

Pimelic acid, butyl octyl ester

Inchi:	InChI=1S/C19H36O4/c1-3-5-7-8-9-13-17-23-19(21)15-12-10-11-14-18(20)22-16-6-4-2/h3
InchiKey:	JUBGJXMNMANFMN-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-358.74	kJ/mol	Joback Method
hf	-925.09	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.184		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1149.10	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	786.70	K	Joback Method
tc	967.58	K	Joback Method
tf	448.21	K	Joback Method
vc	1.147	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.90	J/molxK	786.70	Joback Method
cpg	926.73	J/molxK	816.85	Joback Method
cpg	943.58	J/molxK	846.99	Joback Method
cpg	959.47	J/molxK	877.14	Joback Method
cpg	974.42	J/molxK	907.29	Joback Method
cpg	988.43	J/molxK	937.43	Joback Method
cpg	1001.52	J/molxK	967.58	Joback Method
dvisc	0.0009350	Paxs	448.21	Joback Method

dvisc	0.0004609	Paxs	504.63	Joback Method
dvisc	0.0002619	Paxs	561.04	Joback Method
dvisc	0.0001650	Paxs	617.46	Joback Method
dvisc	0.0001123	Paxs	673.87	Joback Method
dvisc	0.0000812	Paxs	730.29	Joback Method
dvisc	0.0000614	Paxs	786.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393869&Units=SI

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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