

Pimelic acid, butyl heptyl ester

Inchi:	InChI=1S/C18H34O4/c1-3-5-7-8-12-16-22-18(20)14-11-9-10-13-17(19)21-15-6-4-2/h3-16
InchiKey:	CHXQHBOVYXFKIH-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-367.16	kJ/mol	Joback Method
hf	-904.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.794		Crippen Method
mvol	279.360	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	763.82	K	Joback Method
tc	942.53	K	Joback Method
tf	436.94	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.49	J/molxK	763.82	Joback Method
cpg	866.90	J/molxK	793.61	Joback Method
cpg	883.40	J/molxK	823.39	Joback Method
cpg	898.98	J/molxK	853.18	Joback Method
cpg	913.68	J/molxK	882.96	Joback Method
cpg	927.49	J/molxK	912.75	Joback Method
cpg	940.44	J/molxK	942.53	Joback Method
dvisc	0.0010365	Paxs	436.94	Joback Method

dvisc	0.0005169	Paxs	491.42	Joback Method
dvisc	0.0002962	Paxs	545.90	Joback Method
dvisc	0.0001878	Paxs	600.38	Joback Method
dvisc	0.0001284	Paxs	654.86	Joback Method
dvisc	0.0000931	Paxs	709.34	Joback Method
dvisc	0.0000707	Paxs	763.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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