

Pimelic acid, butyl pentyl ester

Inchi:	InChI=1S/C16H30O4/c1-3-5-10-14-20-16(18)12-9-7-8-11-15(17)19-13-6-4-2/h3-14H2,1-2
InchiKey:	SAEDRBKRIXNLAA-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-384.00	kJ/mol	Joback Method
hf	-863.17	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.014		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	718.06	K	Joback Method
tc	894.33	K	Joback Method
tf	414.40	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.60	J/molxK	718.06	Joback Method
cpg	750.17	J/molxK	747.44	Joback Method
cpg	765.92	J/molxK	776.82	Joback Method
cpg	780.87	J/molxK	806.19	Joback Method
cpg	795.02	J/molxK	835.57	Joback Method
cpg	808.37	J/molxK	864.95	Joback Method
cpg	820.95	J/molxK	894.33	Joback Method
dvisc	0.0012551	Paxs	414.40	Joback Method

dvisc	0.0006418	Paxs	465.01	Joback Method
dvisc	0.0003744	Paxs	515.62	Joback Method
dvisc	0.0002405	Paxs	566.23	Joback Method
dvisc	0.0001661	Paxs	616.84	Joback Method
dvisc	0.0001214	Paxs	667.45	Joback Method
dvisc	0.0000927	Paxs	718.06	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=U393809&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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