

Pimelic acid, butyl hexadecyl ester

Inchi:	InChI=1S/C27H52O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-21-25-31-27(29)23-20-18-1
InchiKey:	XNIZORQRQDLLNF-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-291.38	kJ/mol	Joback Method
hf	-1090.21	kJ/mol	Joback Method
hfus	71.26	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.305		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	723.40	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	969.74	K	Joback Method
tc	1199.13	K	Joback Method
tf	538.37	K	Joback Method
vc	1.595	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.71	J/molxK	969.74	Joback Method
cpg	1431.77	J/molxK	1007.97	Joback Method
cpg	1451.97	J/molxK	1046.20	Joback Method
cpg	1470.38	J/molxK	1084.43	Joback Method
cpg	1487.05	J/molxK	1122.66	Joback Method
cpg	1502.06	J/molxK	1160.89	Joback Method
cpg	1515.46	J/molxK	1199.13	Joback Method
dvisc	0.0003585	Paxs	538.37	Joback Method

dvisc	0.0001634	Paxs	610.26	Joback Method
dvisc	0.0000879	Paxs	682.16	Joback Method
dvisc	0.0000532	Paxs	754.06	Joback Method
dvisc	0.0000352	Paxs	825.95	Joback Method
dvisc	0.0000248	Paxs	897.85	Joback Method
dvisc	0.0000185	Paxs	969.74	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=U406552&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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