

Pimelic acid, butyl phenethyl ester

Inchi:	InChI=1S/C19H28O4/c1-2-3-15-22-18(20)12-8-5-9-13-19(21)23-16-14-17-10-6-4-7-11-17
InchiKey:	YCXVOZALRXRDAB-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-246.33	kJ/mol	Joback Method
hf	-688.56	kJ/mol	Joback Method
hfus	44.58	kJ/mol	Joback Method
hvap	78.48	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.066		Crippen Method
mvol	269.690	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2423.00		NIST Webbook
tb	813.38	K	Joback Method
tc	1012.05	K	Joback Method
tf	474.63	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.71	J/molxK	813.38	Joback Method
cpg	835.71	J/molxK	846.49	Joback Method
cpg	850.62	J/molxK	879.60	Joback Method
cpg	864.47	J/molxK	912.71	Joback Method
cpg	877.28	J/molxK	945.83	Joback Method
cpg	889.08	J/molxK	978.94	Joback Method
cpg	899.89	J/molxK	1012.05	Joback Method
dvisc	0.0007727	Paxs	474.63	Joback Method
dvisc	0.0004063	Paxs	531.09	Joback Method

dvisc	0.0002418	Paxs	587.55	Joback Method
dvisc	0.0001576	Paxs	644.00	Joback Method
dvisc	0.0001100	Paxs	700.46	Joback Method
dvisc	0.0000811	Paxs	756.92	Joback Method
dvisc	0.0000623	Paxs	813.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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