Pimelic acid, isobutyl 3-methyl-2-pentyl ester

Inchi: InChI=1S/C17H32O4/c1-6-14(4)15(5)21-17(19)11-9-7-8-10-16(18)20-12-13(2)3/h13-15H
InchiKey: ZFJVGEPFLZXJRQ-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCC(C)C(C)OC(=O)CCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-382.90	kJ/mol	Joback Method
hf	-899.65	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.114		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	739.62	K	Joback Method
tc	922.00	K	Joback Method
tf	380.67	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.48	J/mol×K	739.62	Joback Method
cpg	810.02	J/mol×K	770.02	Joback Method
cpg	826.62	J/mol×K	800.41	Joback Method
cpg	842.29	J/mol×K	830.81	Joback Method
cpg	857.04	J/mol×K	861.21	Joback Method
cpg	870.89	J/mol×K	891.60	Joback Method
cpg	883.84	J/mol×K	922.00	Joback Method
dvisc	0.0021500	Pa×s	380.67	Joback Method

dvisc	0.0008028	Pa×s	440.50	Joback Method
dvisc	0.0003794	Pa×s	500.32	Joback Method
dvisc	0.0002104	Pa×s	560.14	Joback Method
dvisc	0.0001308	Pa×s	619.97	Joback Method
dvisc	0.0000884	Pa×s	679.80	Joback Method
dvisc	0.0000636	Pa×s	739.62	Joback Method

Sources

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=U406594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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