Pimelic acid, isobutyl 2-pentyl ester

Inchi: InChI=1S/C16H30O4/c1-5-9-14(4)20-16(18)11-8-6-7-10-15(17)19-12-13(2)3/h13-14H,5-1
InchiKey: PUQXAGJKRCEXJO-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CCCC(C)OC(=O)CCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-388.88	kJ/mol	Joback Method
hf	-873.73	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.868		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	717.18	K	Joback Method
tc	897.32	K	Joback Method
tf	384.40	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.56	J/mol×K	717.18	Joback Method
cpg	751.53	J/mol×K	747.20	Joback Method
cpg	767.64	J/mol×K	777.23	Joback Method
cpg	782.89	J/mol×K	807.25	Joback Method
cpg	797.29	J/mol×K	837.27	Joback Method
cpg	810.84	J/mol×K	867.29	Joback Method
cpg	823.57	J/mol×K	897.32	Joback Method
dvisc	0.0018907	Pa×s	384.40	Joback Method

dvisc	0.0007981	Pa×s	439.86	Joback Method
dvisc	0.0004087	Pa×s	495.33	Joback Method
dvisc	0.0002395	Pa×s	550.79	Joback Method
dvisc	0.0001547	Pa×s	606.25	Joback Method
dvisc	0.0001076	Pa×s	661.72	Joback Method
dvisc	0.0000791	Pa×s	717.18	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=U393788&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

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