

Pimelic acid, 2-methylpropyl octyl ester

Inchi: InChI=1S/C19H36O4/c1-4-5-6-7-8-12-15-22-18(20)13-10-9-11-14-19(21)23-16-17(2)3/h1-3,11-14,19-21,23-24H,20H2
InchiKey: CQUBGQMLNDMXOQ-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCCOC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-361.18	kJ/mol	Joback Method
hf	-930.37	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	786.26	K	Joback Method
tc	968.16	K	Joback Method
tf	433.21	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.39	J/molxK	786.26	Joback Method
cpg	927.32	J/molxK	816.58	Joback Method
cpg	944.26	J/molxK	846.89	Joback Method
cpg	960.22	J/molxK	877.21	Joback Method
cpg	975.21	J/molxK	907.53	Joback Method
cpg	989.26	J/molxK	937.85	Joback Method
cpg	1002.36	J/molxK	968.16	Joback Method
dvisc	0.0011109	Paxs	433.21	Joback Method

dvisc	0.0005025	Paxs	492.05	Joback Method
dvisc	0.0002693	Paxs	550.89	Joback Method
dvisc	0.0001628	Paxs	609.74	Joback Method
dvisc	0.0001075	Paxs	668.58	Joback Method
dvisc	0.0000759	Paxs	727.42	Joback Method
dvisc	0.0000565	Paxs	786.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393855&Units=SI
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

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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